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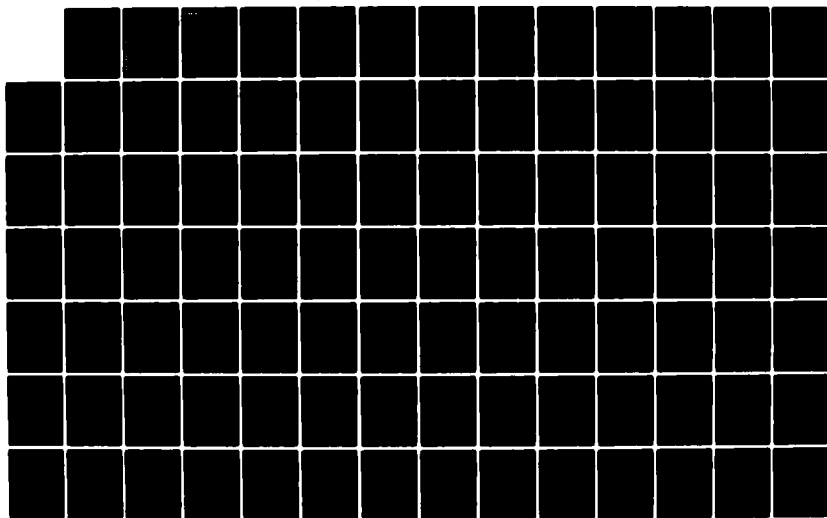
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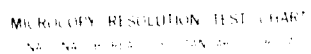
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FLUX-CORRECTED TRANSPORT

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by  
Raafat H. Guirguis

March 21, 1983

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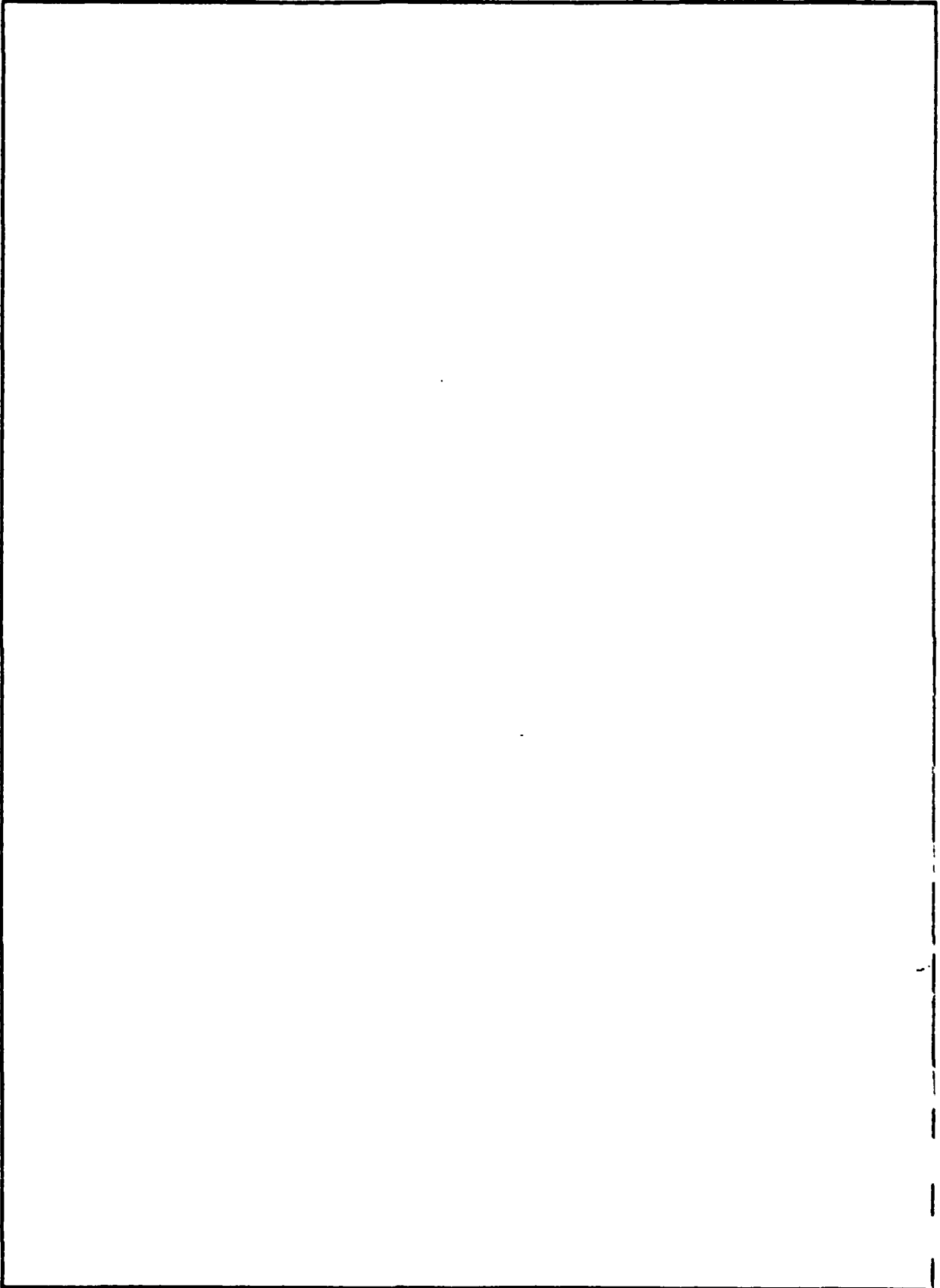
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## TWO-DIMENSIONAL FLUX-CORRECTED TRANSPORT

by

**Raafat H. Guirguis**

**Jaycor, Inc.**

**Alexandria, Virginia**

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## I. INTRODUCTION AND MOTIVATION

A well-documented module ETBFCT for solving generalized continuity equations was presented in NRL Memorandum Report 3237, dated March 1976. The module PRBFCT was also included to treat the case of periodic boundary conditions. In these modules, the cell centers are specified while the cell boundaries are located midway between the centers. In August 1980, JPBFACT, in which the cell boundaries are tracked, was documented.

The above modules are based on the Flux-Corrected Transport (FCT) technique introduced first by Boris and Book.<sup>1</sup> FCT, instead of adhering to an asymptotic ordering, requires positivity, a physical and mathematical property of continuity equations. To assure positivity, the convective stage includes or is supplemented by a large diffusive flux of zeroth order (in  $\epsilon = \frac{u \delta t}{\delta x}$ ). Consequently, an antidiffusive or corrective step has to follow. The two stages together are able to treat steep gradients without generating dispersive ripples. Antidiffusion being a physically (and numerically) unstable process, the corrective flux is limited according to a criterion which may be stated, "The antidiffusion stage should generate no new maxima or minima in the solution, nor should it accentuate already existing extrema."

FCT was shown to be applicable to any finite difference transport scheme and able to improve it.<sup>2</sup> Phenical FCT, a refinement which minimizes residual diffusive errors, was introduced. Clipping and terracing, two nonlinear processes resulting from the flux limiter were discussed. Finally, splitting techniques were recommended to extend FCT to multi-dimensions.

The most detailed error analysis of FCT algorithms was performed in Ref. 3. Low-residual-diffusion and low-phase-error algorithms were derived. An optimal algorithm, Fourier FCT, was introduced.

The requirements for positivity of a general three-point scheme and the antidiffusion flux for a minimum residual diffusion were derived in Ref. 4.

Zalesak<sup>5</sup> provided a general mathematical interpretation of the antidiffusion flux as the difference between a high-order transport scheme and a low-order one. He also described a generalized fully multidimensional flux limiter guaranteeing that the antidiffusion fluxes on all sides of the control volume, acting in concert, do not create any ripples. It was shown that by proper selection of the flux limiter parameters the clipping and terracing phenomena can be reduced.

The goal of the present work is to extend JPBFACT to a fully two-dimensional algorithm, without time splitting, and incorporate the Zalesak flux limiter while still keeping the implementation of the convective, diffusion and antidiffusion processes as physical fluxes.

## II. FOURIER ANALYSIS; DEFINITIONS

A generalized conservation equation can be written in the form:

$$\frac{\partial \rho}{\partial t} + \vec{u} \cdot \nabla \rho = \rho \nabla \cdot \vec{u} + s(\vec{x}, t, \rho, \dots), \quad (1)$$

where  $\vec{u}$  is the velocity vector,  $\rho$  is the generalized density or the transported quantity whose positivity is to be conserved, and  $s$  is a source term including all the remaining terms, i.e., gradients, divergences, body forces, etc.

In the analysis we assume  $s = 0$  and  $\vec{u} = \text{constant}$ . We shall start with the one-dimensional case. Eq. (1) reduces to

$$\frac{\partial \rho}{\partial t} + u_0 \frac{\partial \rho}{\partial x} = 0, \quad (2)$$

whose analytic solution is

$$\rho(x, t) = \rho(x - u_0 t, 0), \quad (3)$$

a rightward-propagating wave with velocity  $u_0$ . Let us Fourier analyze  $\rho(x, t)$  in space, assuming periodic boundary conditions. Assuming an initial distribution of density  $\rho(x, 0) = F(x)$ ,

$$F(x) = \frac{a_0}{2} + \sum_{k=1}^{\infty} (a_k \cos kx + b_k \sin kx), \quad (4a)$$

where  $k$  is assumed to be normalized, i.e.,  $k$  replaces  $\frac{2\pi k}{L}$ . In complex form

$$F(x) = \sum_{k=-\infty}^{\infty} \hat{\rho}_k e^{ikx} \quad (4b)$$

where  $i \equiv \sqrt{-1}$ . From the reality of  $\rho(x, 0)$ , the  $a_k$  and  $b_k$  are real. The quantity  $\hat{\rho}_k$  is related to these by

$$\hat{c}_k = \begin{cases} \frac{a_k - ib_k}{2} & \text{for } k > 0; \\ \frac{a_k + ib_k}{2} & \text{for } k < 0; \\ \frac{a_0}{2} = 0 & \text{for } k = 0. \end{cases} \quad (5)$$

Notice that we could have started the summation in Eq. (4a) from  $k = 0$  since  $\sin 0 = 0$  and  $\cos 0 = 1$ . The zeroth order term would then be  $a_0$ . The form (4a) is preferred, however, since it is compatible with the symmetric formulation of Eqs. (4b) and (5). Then  $\hat{c}_k$  is given by

$$\hat{c}_k = \frac{1}{L} \int_0^L F(x) e^{-ikx} dx. \quad (6)$$

From Eq. (3), the density profile at time  $t$  is given by

$$\rho(x, t) = \sum_{k=-\infty}^{\infty} \hat{c}_k e^{ik(x - u_0 t)} = \sum_{k=-\infty}^{\infty} \hat{c}_k(t) e^{ikx}, \quad (7)$$

where

$$\hat{c}_k(t) = \hat{c}_k e^{-iku_0 t}, \quad (8)$$

showing that each harmonic independently advances uniformly in phase without changing its magnitude (see Fig. 1).

Suppose  $\rho$  is known at all times only as a set of  $N + 1$  quantities  $\rho_j$  on discrete grid points with separation  $\delta x = \frac{L}{N}$ ;  $x_j = j\delta x$  ( $j = 0, 1, \dots, N-1$ ), since  $\rho_0 = \rho_N$ . We can have only  $\frac{N}{2} + 1$  different harmonics. Namely, wave numbers  $(0, 1, \dots, N/2)$  and wavelengths  $(\infty = L/0, \frac{L}{1}, \frac{L}{2}, \dots, \frac{L}{N/2})$  respectively, where we note that the shortest wave length is  $2\delta x$ . Let

$$f(x) = \frac{A_0}{2} + \sum_{k=1}^{N/2} (A_k \cos kx + B_k \sin kx), \quad (9a)$$

or

$$f(x) = \sum_{k=-N/2}^{N/2} \hat{\rho}_k e^{ikx} \quad (9b)$$

(see Fig. 2). We notice in Eq. (9a) that at  $k = N/2$ ,  $\sin kx_j = \frac{2\pi(N/2)}{L} j\delta x = \sin \pi j = 0$ ; hence only  $\cos kx$  is needed at  $k = N/2$ . There are then  $N$  coefficients,  $A_k$  ( $k = 0, \dots, N/2$ ) and  $B_k$  ( $k = 1, 2, \dots, N/2 - 1$ ), which can be determined using  $f(x_j) = \rho_j^0$  ( $j = 0, \dots, N-1$ ), where superscript 0 denotes time  $t = 0$ . Similarly, since for all  $j$ ,  $\exp[i \frac{2\pi}{L} (\frac{-N}{2}) j\delta x] = \exp[i \frac{2\pi}{L} (\frac{N}{2}) j\delta x]$ , Eq. (9b) is rewritten as

$$f(x) = \sum_{k=-N/2+1}^{N/2} \hat{\rho}_k e^{ikx} \quad (9c)$$

Again, we get  $N$  coefficients  $\hat{\rho}_k$  ( $k = -N/2+1, \dots, 0, \dots, N/2$ ). The relation between the  $\hat{\rho}_k$  and  $A_k, B_k$  are given by equations similar to Eq. (5).

Formally,

$$\hat{\rho}_k = \frac{1}{N} \sum_{j=0}^{N-1} \rho_j^0 e^{ikx_j} \quad (10)$$

Eq. (3) predicts the density at time  $t$  as

$$\rho(x, t) = \sum_{k=-N/2+1}^{N/2} \hat{\rho}_k e^{ik(x - u_0 t)} = \sum_{k=-N/2+1}^{N/2} \hat{\rho}_k(t) e^{ikx}$$

where  $\hat{\rho}_k(t) = \hat{\rho}_k e^{-iku_0 t}$ . Since we are only concerned with  $\rho(x_j, t)$ , substituting  $x = x_j = j\delta x$ , we get

$$\rho(x_j, t) = \sum_{k=-N/2+1}^{N/2} \hat{\rho}_k(t) e^{ikj\delta x} \quad (11)$$

If the time is also discretized, let  $t^n \equiv n\delta t$ ,  $\rho_j^n \equiv \rho(x_j, t^n)$ ,  $\hat{\rho}_k^n \equiv \hat{\rho}_k(t^n)$ ,

then

$$\rho_j^n = \sum_{k=-N/2+1}^{N/2} \hat{\rho}_k^n e^{ikj\delta x} \quad (12)$$

where

$$\hat{\rho}_k^n = \hat{\rho}_k e^{-iku_0 n\delta t} \quad (13)$$

If we space-discretize only, after we Fourier analyze the initial density profile  $\rho_j^0$ , i.e., after getting the  $\hat{\rho}_k$  in Eq. (9c), the problem is reduced to that of propagation of the complex harmonics  $e^{ikx}$  ( $k = 0, \dots, N/2$ ). In a nonlinear problem, each harmonic can couple into components of the other harmonics. In the linear problem of Eq. (2), however, each harmonic propagates independently (this is also true if  $u = u(t)$ ). Since the number of spatial points does not change, we can always express the density at any time as a Fourier expansion of the form Eq. (9c). In a nonlinear problem  $\hat{\rho}_k(t)$  is a function of  $(\hat{\rho}_{-N/2+1}, \dots, \hat{\rho}_0, \dots, \hat{\rho}_{N/2})$  at time  $t = 0$ . But in the linear problem  $\hat{\rho}_k(t)$  is only a function of  $\hat{\rho}_k$  as is obvious from Eq. (13). If the time is also discretized, we can then define a transfer function

$$A(k) \equiv \frac{\hat{\rho}_k^{n+1}}{\hat{\rho}_k^n} \quad (14)$$

which is independent of  $n$  if  $u = u_0$  as is obvious from Eq. (13) (analytic solution), yielding

$$A(k) = e^{-iku_0 \delta t} \quad (15)$$

Eq. (12) may be rewritten then as

$$\rho_j^n = \sum_{k=-N/2+1}^{N/2} \hat{\rho}_k [A(k)]^n e^{ikj\delta x}, \quad (16)$$



Denoting the constant  $\frac{u_0 \delta t}{\delta x}$  by  $\varepsilon$  and the dimensionless wave number  $k\delta x$  by  $\beta$ ,  $A(\beta) = e^{-i\beta\varepsilon}$ . The amplification is  $|A(\beta)| = 1$  and the phase shift is  $-\beta\varepsilon$ . Notice that the smallest  $\beta = 0$  and largest  $\beta = \frac{2\pi}{L} \frac{N}{2} \delta x = \pi$ . For a finite-difference scheme applied to the linear problem, each harmonic propagates independently. Consequently, a method equivalent to Fourier-analyzing  $\rho_j^{n+1}$  and  $\rho_j^n$  ( $j = 0, \dots, N-1$ ) and evaluating  $A_k$  from Eq. (14) is to study the propagation of only one harmonic by assuming  $\rho_j^n = \rho^0 e^{ikj\delta x}$ , where  $\rho^0$  is constant. Then

$$A(k) = \frac{\rho_j^{n+1}}{\rho_j^n} \quad (17)$$

By writing  $A(k)$  as

$$A = |A| e^{i\theta}, \quad (18)$$

we define the amplitude (or diffusion) error and the relative phase error as

$$a = |A| - 1 \quad (19a)$$

and

$$R = \frac{(-\theta) - \beta\varepsilon}{\beta\varepsilon} = \frac{-(\theta/\beta)}{\varepsilon} - 1, \quad (19b)$$

respectively. We define a scheme as stable if  $A \leq 1$  (see Fig. 3).

#### Example:

Assuming  $u = \text{const} = u_0$ , the original explicit SHASTA Algorithm can be written as

$$\begin{aligned} \rho_j^{TD} &= \rho_j^n - \frac{\varepsilon}{2}(\rho_{j+1}^n - \rho_{j-1}^n) + \left(\frac{1}{8} + \frac{\varepsilon^2}{2}\right)(\rho_{j+1}^n - 2\rho_j^n + \rho_{j-1}^n) \\ \rho_j^{n+1} &= \rho_j^{TD} - \frac{1}{8}(\rho_{j+1}^{TD} - 2\rho_j^{TD} + \rho_{j-1}^{TD}) \end{aligned} \quad (20)$$

in which we identify  $-\frac{\epsilon}{2}(\rho_{j+1}^n - \rho_{j-1}^n)$  as the net transportive flux, denoted by a superscript T, and  $(\frac{1}{8} + \frac{\epsilon^2}{2})(\rho_{j+1}^n - 2\rho_j^n + \rho_{j-1}^n)$  as the net diffusive flux, denoted by a superscript D, from which we have the notation  $\rho_j^{TD}$ .

Expressing  $\rho_j^{TD}$  as a three-point formula we can write

$$\rho_j^{TD} = [\frac{1}{8} + \frac{\epsilon^2}{2} - \frac{\epsilon}{2}]\rho_{j+1}^n + [1 - 2(\frac{1}{8} + \frac{\epsilon^2}{2})]\rho_j^n + [\frac{1}{8} + \frac{\epsilon^2}{2} + \frac{\epsilon}{2}]\rho_{j-1}^n$$

Each of the quantities in square brackets is  $\geq 0$  for  $|\epsilon| \leq \frac{1}{2}$ , assuring the positivity of  $\rho_j^{TD}$  if  $\rho_j^n \geq 0$ . The positivity requirement will be discussed later in detail. Assuming  $\rho_j^n = \rho^0 e^{ikj\delta x}$ ,

$$\begin{aligned} \rho_j^{TD} &= \rho^0 e^{ikj\delta x} - \frac{\epsilon}{2}(\rho^0 e^{ik(j+1)\delta x} - \rho^0 e^{ik(j-1)\delta x}) \\ &\quad + (\frac{1}{8} + \frac{\epsilon^2}{2})(\rho^0 e^{ik(j+1)\delta x} - 2\rho^0 e^{ikj\delta x} + \rho^0 e^{ik(j-1)\delta x}), \end{aligned}$$

giving

$$\rho_j^{TD}/\rho_j^n = 1 - \frac{\epsilon}{2}(e^{i\beta} - e^{-i\beta}) + (\frac{1}{8} + \frac{\epsilon^2}{2})(e^{i\beta} - 2 + e^{-i\beta}).$$

Denoting the operator  $\frac{e^{i\beta} - e^{-i\beta}}{2} = i \sin \beta$  by  $t$  and  $e^{i\beta} - 2 + e^{-i\beta} = 2(\cos \beta - 1)$  by  $d$ , we have  $\rho_j^{TD} = (1 - \epsilon t + \nu d) \rho_j^n$  where  $\nu \equiv \frac{1}{8} + \frac{\epsilon^2}{2}$ . Then if  $\nu \equiv \frac{1}{8}$ ,  $\rho_j^{n+1} = (1 - \epsilon t + \nu d) \rho_j^n - \nu d(1 - \epsilon t + \nu d) \rho_j^n$ , whence

$$A \equiv \frac{\rho_j^{n+1}}{\rho_j^n} = (1 - \epsilon t + \nu d)(1 - \nu d). \quad (21)$$

We notice that at  $\epsilon = 0$ ,  $A \neq 1$ . In fact,  $A = (1 + \frac{1}{8}d)(1 - \frac{1}{8}d)$ , a deficiency that led to the introduction of a phenical algorithm in Ref. 2, in which the antidiffusion operates on a transported density which is free from any zeroth-order diffusion. Phenical SHASTA is written as

$$\begin{aligned}
\rho_j^T &= \rho_j^n - \frac{\varepsilon}{2}(\rho_{j+1}^n - \rho_{j-1}^n) + \frac{\varepsilon^2}{2}(\rho_{j+1}^n - 2\rho_j^n + \rho_{j-1}^n); \\
\rho_j^{TD} &= \rho_j^T + \frac{1}{8}(\rho_{j+1}^n - 2\rho_j^n + \rho_{j-1}^n); \\
\rho_j^{n+1} &= \rho_j^{TD} - \frac{1}{8}(\rho_{j+1}^T - 2\rho_j^T + \rho_{j-1}^T).
\end{aligned} \tag{22}$$

thus yielding

$$A = (1 - \varepsilon t + \lambda \varepsilon^2 d)(1 - \mu d) + \nu d, \tag{23}$$

where  $\lambda = \frac{1}{2}$ ,  $\nu = \mu = \frac{1}{8}$ , satisfying  $A = 1$  at  $\varepsilon = 0$ .

The importance of phoenicity lies in the fact that the total diffusion through a surface is proportional to the time of diffusion and therefore should vanish as  $\delta t \rightarrow 0$ , i.e.,  $\varepsilon \rightarrow 0$ .

Later, in Ref. 6, ETBFCT and JPBFCCT, based on the scheme

$$\begin{aligned}
\rho_j^T &= \rho_j^n - \frac{\varepsilon}{2}(\rho_{j+1}^n - \rho_{j-1}^n) \\
\rho_j^{TD} &= \rho_j^T + \nu(\rho_{j+1}^n - 2\rho_j^n + \rho_{j-1}^n) \\
\rho_j^{n+1} &= \rho_j^{TD} - \mu(\rho_{j+1}^T - 2\rho_j^T + \rho_{j-1}^T),
\end{aligned} \tag{24}$$

were introduced, yielding

$$A = (1 - \varepsilon t)(1 - \mu d) + \nu d, \tag{25}$$

where  $\nu \equiv \frac{1}{6} + \frac{\varepsilon^2}{3}$  and  $\mu \equiv \frac{1}{6} - \frac{\varepsilon^2}{6}$ . Notice that the zeroth order term is the same in both  $\nu$  and  $\mu$ , thus yielding a residual diffusion  $O(\varepsilon^2)$ , which vanishes as  $\delta t \rightarrow 0$ .

### III. AMPLITUDE AND PHASE ANALYSIS

If in Eq. (18)  $A$  is expressed as  $A = A_R + iA_I$ , where  $R$  stands for real and  $I$  for imaginary, then

$$|A|^2 = A_R^2 + A_I^2, \quad (31a)$$

$$\theta = \tan^{-1}(A_I/A_R). \quad (31b)$$

Equations (31) yield numerical values of  $|A|$  and  $\theta$  for a given  $\beta$ . These should be expanded, however, in a power series in  $\beta$  and plugged into Eqs. (19) to get an estimate of the order of a given scheme. Expanding Eqs. (31) in power series is a huge task. Instead, we use a scheme based on successive differentiation, as follows:

#### PHASE ERRORS

As seen from Eqs. (21), (23), and (25), three-point schemes can be expressed in terms of a transport operator  $t \equiv i \sin \beta$  and a diffusion operator  $d \equiv 2(\cos \beta - 1)$ . In other words,  $A = A(t, d)$  where  $t = t(\beta)$  and  $d = d(\beta)$ . Taking the logarithm of Eq. (18), we obtain  $\log A = \log |A| + i\theta$ , yielding

$$\theta = \text{Im}[\log A]. \quad (33)$$

Expanding  $\theta$  in a power series of  $\beta$ , near  $\beta = 0$ , we have

$$\theta = \theta_0 + \theta'_0 \frac{\beta}{1!} + \theta''_0 \frac{\beta^2}{2!} + \dots$$

where  $( )' \equiv \frac{d( )}{d\beta}$  and the subscript 0 denotes the value at  $\beta = 0$ . Since, from Eq. (33),

$$\frac{d^n \beta}{d\beta^n} \Big|_{\beta=0} = \text{Im} \left\{ \frac{d^n}{d\beta^n} (\log A) \Big|_{\beta=0} \right\},$$

all we need are the derivatives of  $(\log A)$  with respect to  $\beta$ , at  $\beta = 0$ .

First, by direct differentiation we get  $(\log A)' = A'/A$ ,  
 $(\log A)'' = A''/A - (A'/A)^2$  and so on. Noticing that the "consistency" of  
any scheme requires  $A(\beta = 0) = 1$ , we can write

$$(\log A)'_0 = A'_0; \quad (35a)$$

$$(\log A)''_0 = A''_0 - A'^2_0; \quad (35b)$$

$$(\log A)'''_0 = A'''_0 - 3A'_0 A''_0 + 2A'^3_0; \quad (35c)$$

$$(\log A)^{iv}_0 = A^{iv}_0 - 4A'_0 A'''_0 - 3A''^2_0 + 12A'^2_0 A''_0 - 6A'^4_0; \quad (35d)$$

$$\begin{aligned} (\log A)^v_0 = & A^v_0 - 5A'_0 A^{iv}_0 - 10A''_0 A'''_0 + 20A'^2_0 A'''_0 + 30A''^2_0 A'_0 \\ & - 60A'^3_0 A''_0 + 24A'^5_0. \end{aligned} \quad (35e)$$

Next denoting  $\frac{\partial(\cdot)}{\partial t}$  by  $(\cdot)^t$  and  $\frac{\partial}{\partial d}(\cdot)$  by  $(\cdot)^d$ , we get by direct differentiation  $A' = t^t A^t + d^t A^d$ ,  $A'' = t'' A^t + d'' A^d + t'^2 A^{tt} + 2t^t d^t A^{td} + d'^2 A^{dd}$ , and so on. Confining our scope to schemes of first degree in  $t$  (composite transport excluded) and of second degree in  $d$ , we have

$$A^{tt} = 0, A^{tdd} = \text{constant}, \text{ and } A^{ddd} = 0. \quad (36)$$

We obtain then

$$A_0 = 1;$$

$$A'_0 = t^t A^t_0 + d^t A^d_0; \quad (37a)$$

$$A''_0 = t'' A^t_0 + d'' A^d_0 + 2t^t d^t A^{td}_0 + d'^2 A^{dd}_0; \quad (37b)$$

$$A_o''' = t_o''' A_o^t + d_o''' A_o^d + 3(t_o'' d_o' + t_o' d_o'') A_o^{td} + 3d_o' d_o'' A_o^{dd} + 3t_o' d_o''^2 A_o^{tdd}; \quad (37c)$$

$$A_o'^v = t_o'^v A_o^t + d_o'^v A_o^d + (4t_o''' d_o' + 6t_o'' d_o'' + 4t_o' d_o''') A_o^{td} + (4d_o' d_o''' + 3d_o''^2) A_o^{dd} + (12t_o' d_o' d_o'' + 6t_o'' d_o'^2) A_o^{tdd}; \quad (37d)$$

$$A_o^v = t_o^v A_o^t + d_o^v A_o^d + (5t_o'^v d_o' + 10t_o'' d_o'' + 10t_o''' d_o''') A_o^{td} + (5d_o' d_o'^v + 10d_o'' d_o''') A_o^{dd} + (30t_o' d_o' d_o'' + 5t_o' d_o''^2 + 20t_o' d_o' d_o''') + 10t_o''' d_o'^2) A_o^{tdd}. \quad (37e)$$

Going back to the definition of  $t$  and  $d$

$$t_o = 0, t_o' = i, t_o'' = 0, t_o''' = -i, t_o'^v = 0, \text{ and } t_o^v = i, \quad (38a)$$

$$d_o = 0, d_o' = 0, d_o'' = -2, d_o''' = 0, d_o'^v = 2, \text{ and } d_o^v = 0. \quad (38b)$$

Substituting in Eqs. (37), we get

$$A_o = 1;$$

$$A_o' = iA_o^t; \quad (39a)$$

$$A_o'' = -2A_o^d; \quad (39b)$$

$$A_o''' = -i(A_o^t + 6A_o^{td}); \quad (39c)$$

$$A_o'^v = 2(A_o^d + 6A_o^{dd}); \quad (39d)$$

$$A_o^v = i(A_o^t + 30A_o^{td} + 60A_o^{tdd}). \quad (39e)$$

Finally, with Eqs. (30), Eqs. (35) yield

$$(\log A)_0 = 0;$$

$$(\log A)_0' = iA_0^t; \quad (40a)$$

$$(\log A)_0'' = -2A_0^d + (A_0^t)^2; \quad (40b)$$

$$(\log A)_0''' = -iA_0^t(1 - 6A_0^d) - i[6A_0^{td} + 2(A_0^t)^3]; \quad (40c)$$

$$(\log A)_0^{iv} = 12A_0^{dd} + 2(1 - 6A_0^d)[A_0^d - 2(A_0^t)^2] - 6A_0^t[4A_0^{td} + (A_0^t)^3]; \quad (40d)$$

$$(\log A)_0^v = 60iA_0^{tdd} + iA_0^t[1 - 30A_0^d - 60A_0^{dd} + 120(A_0^d)^2] + 20i(A_0^t)^3[1 - 6A_0^d] + 30iA_0^{td}[1 - 4A_0^d + 4(A_0^t)^2] + 24i(A_0^t)^5. \quad (40e)$$

Eqs. (40) invoke the fact that only the odd derivatives of  $\log A$  are imaginary. Therefore, with the use of Eqs. (33) and (34), we get

$$\theta = \frac{(\log A)_0'}{i} \beta + \frac{(\log A)_0'''}{i} \frac{\beta^3}{3!} + \dots \quad (41)$$

Example:

Let us phase-analyze the scheme described by Eqs. (22), i.e., the transfer function of Eq. (23)

$$A = (1 - \epsilon t + \lambda \epsilon^2 d)(1 - \mu d) + \nu d$$

$$\text{where } \nu = \mu = \frac{1}{8} \text{ and } \lambda = \frac{1}{2}.$$

First we notice that it is phoenical:  $A = 1$  at  $\epsilon = 0$ . By direct differentiation,  $A^t = -\epsilon(1 - \mu d)$  and  $A^d = \lambda \epsilon^2(1 - \mu d) - \mu(1 - \epsilon t + \lambda \epsilon^2 d) + \nu$ ;  $A^{td} = \epsilon \mu$ ,  $A^{dd} = -2\lambda \epsilon^2 \mu$ , and  $A^{tdd} = 0$ .

At  $\beta = 0$ ,  $t = 0$  and  $d = 0$ , yielding  $A_O^t = -\epsilon$ , and  $A_O^d = \lambda\epsilon^2 + (v - \mu) = \frac{\epsilon^2}{2}$ ;  
 $A_O^{td} = \epsilon\mu = \frac{\epsilon}{8}$ ,  $A_O^{dd} = -2\lambda\epsilon^2\mu = -\frac{\epsilon^2}{8}$ , and  $A_O^{tdd} = 0$ . Substituting in Eqs. (40),  
 (41), we get

$$\theta = -\epsilon\beta + \frac{1}{6}\left(\frac{1}{4}\epsilon - \epsilon^3\right)\beta^3 + \dots$$

Using Eq. (19b), the relative phase error is found to be

$$R = \frac{1}{6}\left(\frac{1}{4} - \epsilon^2\right)\beta^2 + O(\beta^4),$$

showing that the scheme is second order in phase.

Alternatively, let us derive an expression for  $v$  which renders the scheme of Eqs. (24) fourth-order in phase. Upon differentiating the transfer function  $A = (1 - \epsilon t)(1 - \mu d) + vd$  we get, when we substitute  $\beta = 0$ ,

$$A_O^t = -\epsilon; \text{ and } A_O^d = v - \mu;$$

$$A_O^{td} = \epsilon\mu, A_O^{dd} = 0, \text{ and } A_O^{tdd} = 0, \quad (42)$$

which with Eqs. (39a) through (39c) gives

$$A_O' = -i\epsilon$$

$$A_O'' = -2(v - \mu)$$

$$A_O''' = -i(-\epsilon + 6\epsilon\mu). \quad (43)$$

Substituting in Eq. (35c), we obtain

$$\text{Im}(\log A)_O''' = \epsilon(1 - 6\mu) - 6\epsilon(v - \mu) + 2\epsilon^3 = \epsilon(1 - 6v + 2\epsilon^2).$$

To reduce the coefficient of  $\beta^2$  in the  $R$  expansion to zero we require

$(\log A)_O''' = 0$ , yielding

$$v = \frac{1}{6} + \frac{\epsilon^2}{3} \quad (44)$$



## AMPLITUDE ANALYSIS

Denote the complex conjugate by a bar on top:

$$|A|^2 = A \bar{A}. \quad (45)$$

Since  $\frac{d^n}{d\beta^n} \overline{(\quad)} = \overline{\frac{d^n(\quad)}{d\beta^n}}$ , we get by successive differentiation of Eq. (45)

$$(|A|^2)_0 = 1;$$

$$(|A|^2)'_0 = A'_0 \bar{A}_0 + A_0 \bar{A}'_0; \quad (46a)$$

$$(|A|^2)''_0 = A''_0 \bar{A}_0 + 2A'_0 \bar{A}'_0 + A_0 \bar{A}''_0; \quad (46b)$$

$$(|A|^2)'''_0 = A'''_0 \bar{A}_0 + 3A''_0 \bar{A}'_0 + 3A'_0 \bar{A}''_0 + A_0 \bar{A}'''_0; \quad (46c)$$

$$(|A|^2)^{iv}_0 = A^{iv}_0 \bar{A}_0 + 4A'''_0 \bar{A}'_0 + 6A''_0 \bar{A}''_0 + 4A'_0 \bar{A}'''_0 + A_0 \bar{A}^{iv}_0. \quad (46d)$$

Noticing from Eqs. (39) that the odd derivatives of A are pure imaginary while the even ones are pure real.

$$A_0 = + \bar{A}_0 = 1;$$

$$A'_0 = - \bar{A}'_0;$$

$$A''_0 = + \bar{A}''_0;$$

$$A'''_0 = - \bar{A}'''_0; \quad (47)$$

and

$$A^{iv}_0 = + \bar{A}^{iv}_0.$$

Substituting in Eqs. (46), we get

$$(|A|^2)_0 = 1; \quad (48a)$$

$$(|A|^2)'_0 = 0; \quad (48b)$$

$$(|A|^2)''_0 = 2[A''_0 + (\frac{A'_0}{i})^2]; \quad (48c)$$

$$(|A|^2)'''_0 = 0; \quad (48d)$$

$$(|A|^2)^{iv}_0 = 2[A^{iv}_0 + 4(\frac{A'_0}{i})(\frac{A'''}_0) + 3(A''_0)^2], \quad (48e)$$

where we notice that the odd derivatives vanish. Accordingly,  $|A|^2$  can be expanded as

$$|A|^2 = 1 + (|A|^2)''_0 \frac{\beta^2}{2!} + (|A|^2)^{iv}_0 \frac{\beta^4}{4!} + \dots \quad (49)$$

Example:

Let us derive an expression for  $\mu$  to render the diffusion error of ETBFCT fourth order. Substituting Eqs. (42) into Eq. (39d), we find

$$A^{iv}_0 = 2(\nu - \mu), \quad (50)$$

Using Eqs. (43) with (48), we obtain  $(|A|^2)''_0 = 2[-2(\nu - \mu) + \epsilon^2]$ , which has to vanish for a fourth-order diffusion, yielding

$$\nu - \mu = \frac{\epsilon^2}{2}. \quad (51)$$

Solving Eqs. (44) and (51), we have  $\mu = \frac{1-\epsilon^2}{6}$ , whence  $\frac{A'_0}{i} = -\epsilon$ ,  $A''_0 = -\epsilon^2$ ,

$\frac{A'''}_0 = \epsilon(1 - 6\mu) = \epsilon^3$ , and  $A^{iv}_0 = \epsilon^2$ . We can then write

$$(|A|^2)^{iv}_0 = 2[\epsilon^2 + 4(-\epsilon)(\epsilon^3) + 3\epsilon^4] = 2\epsilon^2(1 - \epsilon^2),$$

which when substituted into Eq. (49) gives

$$|A|^2 = 1 \frac{\varepsilon^2}{12} (1 - \varepsilon^2) \beta^4 + O(\beta^6), \quad (52)$$

showing a slight instability near  $\beta = 0$  (the coefficient of  $\beta^4$  is positive).

A warning is in order at this point. Although a positive coefficient of the leading term in the expansion implies unstable behavior, a negative one does not guarantee a stable scheme, since the expansion is valid only near  $\beta = 0$ .

Figure 4 shows the amplification  $|A|$  versus  $\beta$ . We notice a maximum value of  $|A| = 1.0018$  at  $\beta = 53.668^\circ \pm 0.001$  for  $\varepsilon = \frac{1}{2}$ . We can get rid of the potential instability by using a slightly different expression for  $u$ ,

$$u = \frac{1}{6} - \alpha \frac{\varepsilon^2}{6}. \quad (53)$$

By trial and error,  $\alpha$  was found to be  $\geq 1.056$ . The dashed line in Fig. 4 shows the resulting amplification for  $\alpha = 1.056$ . The maximum value of  $|A|$  becomes 0.999998 at  $\beta = 45.775^\circ \pm 0.001$ . Since the phase error depends on  $v$  only, the resulting scheme is still fourth-order in phase error. The zeroth-order antidiffusion being kept at  $\frac{1}{6}$ , phoenicity is preserved, i.e., the residual diffusion is  $O(\varepsilon^2)$ . Later, a modified algorithm which is stable and has sixth-order diffusion and fourth-order phase error is described.

## IV. POSITIVITY AND ANTIDIFFUSION

The concept underlying FCT is "positivity." This means that the sign of the dependent variable must be preserved under the influence of convection alone. Source terms can alter the sign. Positivity is particularly important near steep gradients where the convective fluxes tend to make the transported quantity undershoot or overshoot. Positivity is ensured by supplementing the convective step with a large diffusive flux of zeroth order in  $\Delta t$ . For example, in the scheme of Eq. (24), consider the transport step alone,

$$\rho_j^T = \rho_j^n - \frac{\varepsilon}{2}(\rho_{j+1}^n - \rho_{j-1}^n),$$

applied to the discontinuities of Fig. 5(a) and (b), where  $\varepsilon = +1/2$ . The negative density in Fig. 5(a) and overshoot in Fig. 5(b) are obviously major errors. By supplying enough diffusion,

$$\rho_j^{TD} = \rho_j^T + \left(\frac{1}{6} + \frac{\varepsilon^2}{3}\right)(\rho_{j+1}^n - 2\rho_j^n + \rho_{j-1}^n),$$

we see the negative density in Fig. 5(a) disappear, as does the overshoot in Fig. 5(b). Formally, in the expression

$$\rho_j^{TD} = \left[1 - 2\left(\frac{1}{6} + \frac{\varepsilon^2}{3}\right)\right] \rho_j^n + \left[\left(\frac{1}{6} + \frac{\varepsilon^2}{3}\right) - \frac{\varepsilon}{2}\right] \rho_{j+1}^n + \left[\left(\frac{1}{6} + \frac{\varepsilon^2}{3}\right) + \frac{\varepsilon}{2}\right] \rho_{j-1}^n,$$

the quantities in square brackets are all  $\geq 0$  for  $|\varepsilon| \leq 1/2$ , therefore ensuring positivity of  $\rho_j^{TD}$  as long as  $\rho_j^n \geq 0$ .

A side benefit of the zeroth-order term is more accurate propagation i.e., high-order phase preservation. As seen from Eq. (44), selecting  $\nu = \frac{1}{6} + \frac{\varepsilon^2}{3}$  assures a fourth-order phase error.

A byproduct of this large added diffusion is antidiffusion, which is needed to extract at least the zeroth order part. This leaves a residual diffusion  $O(\varepsilon^2)$  near almost uniform distributions. Near steep gradients,

antidiffusion fluxes have to be reduced enough to maintain the positivity of  $\rho^{TD}$ . This process is called correction of fluxes, and gives rise to the name "flux-corrected transport." In the case of a discontinuity, the local antidiffusion flux is cancelled completely. This trimming means that the amplitude no longer has the order of accuracy derived above. But near steep gradients the concept of order is meaningless anyway. On the other hand, Eq. (44) is independent of  $\mu$ . The fourth order phase error is therefore assured regardless of the antidiffusion fluxes. Specifically, "the antidiffusion stage should generate no new maxima or minima in the solution, nor should it accentuate already existing extrema" (Ref. 1).

The first mathematical formulation of the above statement was given in connection with explicit SHASTA,<sup>1</sup>

$$\rho_j^{TD} = \rho_j^n - \frac{\varepsilon}{2}(\rho_{j+1}^n - \rho_{j-1}^n) + \left(\frac{1}{8} + \frac{\varepsilon^2}{2}\right)(\rho_{j+1}^n - 2\rho_j^n + \rho_{j-1}^n) \quad (61a)$$

$$\rho_j^{n+1} = \rho_j^{TD} - (f_{j+\frac{1}{2}}^C - f_{j-\frac{1}{2}}^C) \quad (61b)$$

The corrected antidiffusion flux,

$$f_{j+\frac{1}{2}}^C = \text{sign } \Delta_{j+\frac{1}{2}} \cdot \max \{0, \min [\Delta_{j-\frac{1}{2}} \cdot \text{sign } \Delta_{j+\frac{1}{2}}, \frac{1}{8} |\Delta_{j+\frac{1}{2}}|, \Delta_{j+\frac{3}{2}} \cdot \text{sign } \Delta_{j+\frac{1}{2}}]\} \quad (62)$$

is the corrected form of the raw flux

$$f_{j+\frac{1}{2}} \equiv \frac{1}{8} \Delta_{j+\frac{1}{2}} \equiv \frac{1}{8}(\rho_{j+1}^{TD} - \rho_j^{TD}), \quad (63)$$

which in this scheme is always in the same direction as the gradient in  $\rho^{TD}$ . There are eight different possible cases, shown schematically in Fig. 6. Cases 5-8 are mirror images of 1-4, respectively.

Equation (62) will cancel an antidiffusion flux whenever it would lead to accentuate a maximum or a minimum, as illustrated in Fig. 6, and will trim it enough not to generate a new maximum or minimum whenever it is not cancelled.

Later in Ref. 2 the raw antidiffusion fluxes were evaluated using  $\rho_j^T$  in the raw flux  $f_{j+1/2} \equiv \frac{1}{8}(\rho_{j+1}^T - \rho_j^T)$ , where

$$\rho_j^T \equiv \rho_j^n - \frac{\varepsilon}{2}(\rho_{j+1}^n - \rho_{j-1}^n) + \frac{\varepsilon^2}{2}(\rho_{j+1}^n - 2\rho_j^n + \rho_{j-1}^n).$$

The corrected flux is expressed as

$$f_{j+1/2}^C = \text{sign } f_{j+1/2} \cdot \max \{0, \min [|\Delta_{j-1/2}| \cdot \text{sign } f_{j+1/2}, |f_{j+1/2}|, \Delta_{j+3/2} \cdot \text{sign } f_{j+1/2}]\}, \quad (64)$$

where we get sixteen possible cases (twice as many as before, depending whether  $f_{j+1/2}$  is parallel to  $\Delta_{j+1/2}$  or opposite to it). In Fig. 7 we consider only those cases when  $f_{j+1/2}$  is positive, since the other cases are their mirror images.

Again, the flux is cancelled whenever it would accentuate a maximum or minimum. But it is also cancelled in cases 6-8 where it would not in general cause any problems, an unnecessary action. This is due to the fact that  $f_{j+1/2}$  is corrected independently of  $f_{j-1/2}$  and  $f_{j+3/2}$ .

Zalesak<sup>5</sup> reexpressed the role of the flux limiter as "guaranteeing that the two antidiffusion fluxes associated with each cell, acting in concert, should not create any ripples." The mathematical formula

implementing the above statement is described for 1-D schemes by the following steps:

$$\begin{aligned}
 P_j^+ &\equiv \text{sum of antidiffusive fluxes "into" grid point } j \\
 &= \max(0, f_{j-\frac{1}{2}}) - \min(0, f_{j+\frac{1}{2}})
 \end{aligned} \tag{65}$$

$$Q_j^+ \equiv (c_j^{\max} - \rho_j^{\text{TD}}) \tag{66}$$

$$R_j^+ \equiv \begin{cases} \min(1, Q_j^+/P_j^+) & \text{if } P_j^+ > 0 \\ 0 & \text{if } P_j^+ = 0. \end{cases} \tag{67}$$

Similarly,

$$\begin{aligned}
 P_j^- &\equiv \text{sum of antidiffusive fluxes "out of" grid point } j \\
 &= \max(0, f_{j+\frac{1}{2}}) - \min(0, f_{j-\frac{1}{2}})
 \end{aligned} \tag{68}$$

$$Q_j^- \equiv (c_j^{\text{TD}} - \rho_j^{\min}) \tag{69}$$

$$R_j^- \equiv \begin{cases} \min(1, Q_j^-/P_j^-) & \text{if } P_j^- > 0 \\ 0 & \text{if } P_j^- = 0, \end{cases} \tag{70}$$

where  $\rho_j^{\max}$  and  $\rho_j^{\min}$  are the upper and lower bounds on  $\rho_j^{n+1}$ , respectively, which ensure that no ripples form at grid point  $j$ . Defining the correction ratio

$$C_{j+\frac{1}{2}} \equiv \begin{cases} \min(R_{j+1}^+, R_j^-) & \text{if } f_{j+\frac{1}{2}} > 0 \\ \min(R_j^+, R_{j+1}^-) & \text{if } f_{j+\frac{1}{2}} < 0. \end{cases} \tag{71}$$

we set

$$f_{j+\frac{1}{2}}^c = C_{j+\frac{1}{2}} f_{j+\frac{1}{2}}. \tag{72}$$

A conservative choice for  $\rho_j^{\max}$  and  $\rho_j^{\min}$  is

$$\begin{aligned}\rho_j^{\max} &= \max (\rho_{j-1}^{\text{TD}}, \rho_j^{\text{TD}}, \rho_{j+1}^{\text{TD}}) \\ \rho_j^{\min} &= \min (\rho_{j-1}^{\text{TD}}, \rho_j^{\text{TD}}, \rho_{j+1}^{\text{TD}}).\end{aligned}\quad (73)$$

This choice will guarantee that no maxima or minima form other than those already existing in the  $\rho^{\text{TD}}$  distribution. The flux limiter of Eq. (64), however, not only guarantees no ripples, but it also cancels the flux in cases 6-8 of Fig. 1. To reproduce the results of Eq. (64), one should apply the extra limiter

$$\begin{aligned}f_{j+\frac{1}{2}}^{\text{C}} &= 0 \\ \text{if } (f_{j+\frac{1}{2}} \cdot \Delta_{j+\frac{1}{2}} < 0 \text{ and } (f_{j+\frac{1}{2}} \cdot \Delta_{j+3/2} < 0 \text{ or } f_{j+\frac{1}{2}} \cdot \Delta_{j-\frac{1}{2}} < 0))\end{aligned}\quad (74)$$

before Eq. (64).

An extension of Eq. (64) to more than one dimension, however, cannot guarantee that there will be no ripples since it lacks knowledge of  $f_{j+3/2}$  and  $f_{j-\frac{1}{2}}$  when correcting  $f_{j+\frac{1}{2}}$ . We are left then with only one safe solution, which is the extension of Eqs. (65) to (74) to multidimensions. Now, going back to Eq. (73), a more tolerant choice would be

$$\begin{aligned}\rho_j^{\max} &= \max \{ \max (\rho_{j-1}^{\text{TD}}, \rho_{j-1}^{\text{n}}), \max (\rho_j^{\text{TD}}, \rho_j^{\text{n}}), \max (\rho_{j+1}^{\text{TD}}, \rho_{j+1}^{\text{n}}) \}; \\ \rho_j^{\min} &= \min \{ \min (\rho_{j-1}^{\text{TD}}, \rho_{j-1}^{\text{n}}), \min (\rho_j^{\text{TD}}, \rho_j^{\text{n}}), \min (\rho_{j+1}^{\text{TD}}, \rho_{j+1}^{\text{n}}) \}.\end{aligned}\quad (75)$$

This choice will partially avoid the clipping associated with the flux correction of Eq. (73), as explained in Ref. 5. In summary, by calibrating  $(\rho_j^{\max}, \rho_j^{\min})$  using a guaranteed positive profile, positivity is still preserved after the antidiffusion step is performed.



Now that we have all the definitions and tools necessary for analysis,  
let us go back to analyzing schemes.

# V. A STABLE SIXTH-ORDER DIFFUSION ERROR FOURTH-ORDER PHASE ERROR SCHEME

As mentioned earlier, ETBFCT can be made stable by using  $u = 1/6 - \alpha \frac{\epsilon^2}{6}$ , where  $\alpha \geq 1.056$ . Then

$$(|A|^2)_0'' = 2[-2(v - \mu) + \epsilon^2] = 2[-2(\frac{2+\alpha}{6}) + 1]\epsilon^2,$$

yielding

$$|A|^2 = 1 - (\frac{\alpha-1}{3})\epsilon^2\beta^2 + O(\beta^4), \quad (81)$$

which gives for  $\alpha = 1.056$

$$|A|^2 = 1 - \frac{0.056}{3}\epsilon^2\beta^2 + O(\beta^4),$$

thus giving the scheme a small second-order error, but leaving it essentially fourth order in amplitude.

An alternative is to add a small phenical diffusion  $O(\epsilon^2)$  to  $\phi^T$ .

We get then

$$\begin{aligned} \phi_j^T &= \phi_j^n - \frac{\epsilon}{2}(\phi_{j+1}^n - \phi_{j-1}^n) + \lambda\epsilon^2(\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n); \\ \phi_j^{TD} &= \phi_j^T + v(\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n); \\ \phi_j^{n+1} &= \phi_j^{TD} - \mu(\phi_{j+1}^T - 2\phi_j^T + \phi_{j-1}^T). \end{aligned} \quad (82)$$

Assuming  $\phi_j^n = \phi^0 e^{ikj\delta x}$ ,

$$A = (1 - \epsilon t + \lambda\epsilon^2 d)(1 - \mu d) + v d, \quad (83)$$

where  $t \equiv i \sin \beta$  and  $d \equiv 2(\cos \beta - 1)$ . Following the method of analysis described above, we write

$$A_O^t = -\epsilon, A_O^d = (\nu + \lambda\epsilon^2) - \mu,$$

$$A_O^{td} = \epsilon\mu, A_O^{dd} = -2\lambda\epsilon^2\mu, \text{ and } A_O^{tdd} \approx 0$$

Then

$$A_O' = -i\epsilon;$$

$$A_O'' = -2[(\nu + \lambda\epsilon^2) - \mu];$$

$$A_O''' = -i[-\epsilon + 6\epsilon\mu];$$

$$A_O^{iv} = 2[\nu + \lambda\epsilon^2 - \mu - 12\lambda\epsilon^2\mu];$$

For a fourth-order diffusion error,

$$(|A|^2)_O'' = 2[-2(\nu + \lambda\epsilon^2 - \mu) + \epsilon^2] = 0,$$

yielding

$$\nu + \lambda\epsilon^2 - \mu = \frac{\epsilon^2}{2}.$$

Going back to the  $A_O''$ ,  $A_O^{iv}$  expressions, we can rewrite them as

$$A_O'' = -\epsilon^2,$$

$$A_O^{iv} = \epsilon^2 - 24\lambda\epsilon^2\mu.$$

For a fourth-order phase error

$$\begin{aligned} (\log A)_O''' &= -i[-\epsilon + 6\epsilon\mu] - 3(-i\epsilon)(-2)(\nu + \lambda\epsilon^2 - \mu) + 2(-i\epsilon)^3 \\ &= i\epsilon[1 - 6(\nu + \lambda\epsilon^2) + 2\epsilon^2] = 0, \end{aligned}$$

yielding

$$\nu + \lambda\epsilon^2 = 1/6 + \epsilon^2/3,$$

which gives

$$\nu = 1/6 - \epsilon^2/6$$

We can then rewrite  $A_{\circ}'''$  and  $A_{\circ}^{IV}$  as

$$A_{\circ}''' = i\epsilon^3,$$

$$A_{\circ}^{IV} = \epsilon^2 - 4\lambda\epsilon^2(1 - \epsilon^2).$$

Checking,

$$(|A|^2)_{\circ}^{IV} = 2[\epsilon^2 - 4\lambda\epsilon^2(1 - \epsilon^2) - 4\epsilon^4 + 3\epsilon^4]$$

$$= 2[1 - 4\lambda]\epsilon^2(1 - \epsilon^2).$$

showing that we can make the scheme sixth-order in diffusion by selecting

$$\lambda = 1/4.$$

In summary,

$$\nu = 1/6 + \epsilon^2/12, \mu = 1/6 - \epsilon^2/6, \lambda = 1/4. \quad (84)$$

Again, we have to check  $^{TD}$ :

$$\rho_j^{TD} = [1 - 2(\frac{1}{6} + \frac{\epsilon^2}{2})]\rho_j^n + [\frac{1}{6} + \frac{\epsilon^2}{3} - \frac{\epsilon}{2}]\rho_{j+1}^n + [\frac{1}{6} + \frac{\epsilon^2}{3} + \frac{\epsilon}{2}]\rho_{j-1}^n.$$

Each quantity in square brackets is  $\geq 0$  if  $|\epsilon| \leq 1/2$ , yielding  $\rho_j^{TD} \geq 0$  if

$\rho_j^n \geq 0$ , thus ensuring positivity. Figure 8 shows  $|A|$  and  $R$  versus  $\beta$ .

Finally, we note that this is still a 5-point scheme.

## VI. EXTENSION TO HIGHER ORDERS IN DIFFUSION AND PHASE ERRORS

We seek a combination of transport operator  $t(t \equiv i \sin \beta)$  and diffusion operator  $d(d \equiv 2(\cos \beta - 1))$  which approaches the analytic solution up to a prescribed order of  $\beta$ . Since the transfer function of the analytic solution is expressed as  $A = e^{-i\beta\epsilon}$ ,

$$A = \cos \beta\epsilon - i \sin \beta\epsilon \quad (85)$$

or

$$A_I = -\sin \beta\epsilon$$

$$A_R = \cos \beta\epsilon. \quad (86)$$

Now, we write  $\sin \beta\epsilon$  as

$$\sin \beta\epsilon = \sin \beta [A_0 + A_1(1 - \cos \beta) + A_2(1 - \cos \beta)^2 + \dots], \quad (87)$$

where  $A_0, A_1, A_2, \dots$  are determined such as to make the series expansion of both sides of Eq. (87) agree up to a prescribed order of  $\beta$ . In other words, the derivatives of both sides with respect to  $\beta$  at  $\beta = 0$  have to be equal. We get the following system of algebraic equations:

$$\begin{bmatrix} \epsilon \\ -\epsilon^3 \\ \epsilon^5 \\ . \\ . \\ . \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & \dots \\ -1 & 3 & 0 & 0 & \dots \\ 1 & -15 & 30 & 0 & \dots \\ . & . & . & . & . \\ . & . & . & . & . \\ . & . & . & . & . \end{bmatrix} \begin{bmatrix} A_0 \\ A_1 \\ A_2 \\ . \\ . \\ . \end{bmatrix} \quad (88)$$

solved by "forward substitution" since the matrix of coefficients is already

"left-triangular." We solve for  $A_0$  first, then for  $A_1$ , etc. We get

$$A_0 = \varepsilon, A_1 = \frac{\varepsilon(1-\varepsilon^2)}{3}, A_2 = \frac{\varepsilon(4-\varepsilon^2)(1-\varepsilon^2)}{30}, \dots \quad (89)$$

As for the construction of the matrix, the first column is the odd derivatives of  $\sin \beta$ , the second, those of  $\sin \beta(1 - \cos \beta)$ , the third, those of  $\sin \beta(1 - \cos \beta)^2, \dots$  and so on, all at  $\beta = 0$ . We notice that the even derivatives are all zero. To get these, let  $\phi \equiv 1 - \cos \beta$ , and define  $K$  recursively  $K_{i+1} \equiv K_i \phi$  where  $K_0 \equiv \sin \beta$ . If we have the derivatives of  $K_i$ , those of  $K_{i+1}$  will be

$$\begin{aligned} K_{i+1} &= K_i \phi; \\ K'_{i+1} &= K'_i \phi + K_i \phi'; \\ K''_{i+1} &= K''_i \phi + 2K'_i \phi' + K_i \phi'', \end{aligned} \quad (90)$$

and so on. Generally if  $( )^{(n)} \equiv \frac{d^n ( )}{d\beta^n} \Big|_{\beta=0}$  and  $( )^{(0)} \equiv ( )$ , we get

$$K_{i+1}^{(n)} = \sum_{m=0}^n \binom{n}{m} K_i^{(m)} \phi^{(n-m)} \quad (91)$$

where  $\binom{n}{m} = \frac{n!}{(n-m)!m!}$ . All we need then is the derivatives of  $K_0 \equiv \sin \beta$  and  $\phi \equiv 1 - \cos \beta$  at  $\beta = 0$ ; namely,

$$\begin{aligned} K_0 &= 0, K'_0 = 1, K''_0 = 0, K'''_0 = -1, \dots, \text{ and} \\ \phi &= 0, \phi' = 0, \phi'' = 1, \phi''' = 0, \phi^{(4)} = -1, \dots \end{aligned} \quad (92)$$

Now, we write  $\cos \beta \varepsilon$  as

$$\cos \beta \varepsilon = B_0 + B_1(1 - \cos \beta) + B_2(1 - \cos \beta)^2 + \dots \quad (93)$$

where  $B_0, B_1, B_2, \dots$ , are determined such as to make the series expansion of both sides of Eq. (93) agree up to a prescribed order of  $\beta$ . In this case

$$K_0 = 1, K_0' = K_0'' = K_0''' = \dots = 0. \quad (94)$$

Using Eq. (91), we get

$$\begin{bmatrix} 1 \\ -\epsilon^2 \\ \epsilon^4 \\ . \\ . \\ . \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & \dots \\ 0 & 1 & 0 & 0 & \dots \\ 0 & -1 & 6 & 0 & \dots \\ . & . & . & . & . \\ . & . & . & . & . \\ . & . & . & . & . \end{bmatrix} \begin{bmatrix} B_0 \\ B_1 \\ B_2 \\ . \\ . \\ . \end{bmatrix} \quad (95)$$

where we notice again a "left-triangular" coefficients matrix. By "forward substitution" we obtain

$$B_0 = 1, B_1 = -\epsilon^2, B_2 = \frac{-\epsilon^2}{6} (1 - \epsilon^2) \dots \quad (96)$$

Obviously, we can get Eq. (93) by differentiating Eq. (87) and vice versa, but we need then to continue the expansion one more term and use trigonometric identities. The direct approach followed is, however, preferred, since it enforces a given form on the expansion which is in no way unique, as explained below.

Noticing that  $\sin \beta = t/i$  and  $1 - \cos \beta = -d/2$ , we can write a sixth-order diffusion error, sixth-order phase error scheme, for example, as

$$A_R = 1 + \frac{\varepsilon^2}{2} d - \frac{\varepsilon^2}{24} (1 - \varepsilon^2) d^2$$

$$iA_1 = -\varepsilon t \left[ 1 - \frac{1 - \varepsilon^2}{6} d + \frac{1 - \varepsilon^2}{30} \left( 1 - \frac{\varepsilon^2}{4} \right) d^2 \right]. \quad (97)$$

If we stop at  $A_1$ ,  $B_1$ , we get ETBFCT, which has fourth-order diffusion and phase error. Although  $t$  and  $d$  are both three-point operators,  $td^2$  is a seven-point formula. An important conclusion follows: We need three points for a second-order diffusion and phase error, five points for a fourth-order error, and so on, adding two points at a time. We can, however, get sixth-order diffusion and fourth-order phase accuracy with only five points since we have to match the sum  $|A|^2 = A_I^2 + A_R^2$  up to a prescribed order of  $\beta$  and not  $A_I$  and  $A_R$  separately. Scheme (82) is an example. Alternatively one can construct a scheme with fourth-order diffusion and sixth-order phase accuracy using only five points since we have to expand  $\tan^{-1} \frac{A_I}{A_R}$ , not  $A_I$  and  $A_R$  separately.

Before implementing Eq. (97), it is important to emphasize that the expansion is not unique. For example, we can use the expansions

$$\sin \beta \varepsilon = \sin \beta [A_0 + A_1(1 - \cos \beta) + A_2(1 - \cos 2\beta) + \dots],$$

$$\cos \beta \varepsilon = B_0 + B_1(1 - \cos \beta) + B_2(1 - \cos 2\beta) + \dots \quad (98)$$

We get then

$$\begin{bmatrix} \varepsilon \\ -\varepsilon^3 \\ \varepsilon^5 \\ . \\ . \\ . \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & \dots \\ -1 & 3 & 12 & \dots \\ 1 & -15 & -120 & \dots \\ . & . & . & . \\ . & . & . & . \\ . & . & . & . \end{bmatrix} \begin{bmatrix} A_0 \\ A_1 \\ A_2 \\ . \\ . \\ . \end{bmatrix} \quad (99)$$



and

$$\begin{bmatrix} 1 \\ -\varepsilon^2 \\ \varepsilon^4 \\ . \\ . \\ . \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & \dots \\ 0 & 1 & 4 & \dots \\ 0 & -1 & -16 & \dots \\ . & . & . & . \\ . & . & . & . \\ . & . & . & . \end{bmatrix} \begin{bmatrix} B_0 \\ B_1 \\ B_2 \\ . \\ . \\ . \end{bmatrix}$$

By solving the two systems (99), (100), we obtain

$$A_0 = \varepsilon, A_1 = \frac{\varepsilon(9 - \varepsilon^2)(1 - \varepsilon^2)}{15}, A_2 = \frac{-\varepsilon(4 - \varepsilon^2)(1 - \varepsilon^2)}{60} \quad (100)$$

and

$$B_0 = 1, B_1 = \frac{-\varepsilon^2}{3}(4 - \varepsilon^2), B_2 = \frac{\varepsilon^2}{2}(1 - \frac{\varepsilon^2}{6}). \quad (101)$$

We notice that the matrices are full and the coefficients ( $A_1, A_2, \dots$ ); ( $B_1, B_2, \dots$ ) are more complex in form than the corresponding coefficients Eq. (89), (96). Moreover, they change if the expansion is extended to higher order. The operator  $(1 - \cos 2\theta)$  results from a five-point formula; namely,  $\rho_{j+2} - 2\rho_j + \rho_{j-2}$ . It is abandoned therefore in favor of the three-point operator formula of Eq. (97) since the latter requires knowledge of only one point outside the boundary.

We rewrite Eq. (97) as

$$\begin{aligned} A \equiv A_R + iA_I = & -\varepsilon t \left\{ 1 - \left( \frac{1 - \varepsilon^2}{6} \right) d + \left( \frac{1 - \varepsilon^2}{6} \right) \frac{1}{5} \left( 1 - \frac{\varepsilon^2}{4} \right) d^2 \right\} \\ & + \left\{ 1 + \frac{\varepsilon^2}{2} d - \frac{\varepsilon^2}{4} \left( \frac{1 - \varepsilon^2}{6} \right) d^2 \right\}. \end{aligned}$$

Noting that  $\rho^{n+1} = A\rho^n$ , let us collect the terms in such a way as to ensure positivity at every step. First,  $(-\epsilon t)\rho^n = \rho^T - \rho^n$  where

$$\rho_j^T = \rho_j^n - \frac{\epsilon}{2}(\rho_{j+1}^n - \rho_{j-1}^n).$$

Then

$$\begin{aligned} \rho^{n+1} = \rho^n + \left(\frac{\epsilon^2}{2}d\right)\rho^n - \left\{\left(\frac{1-\epsilon^2}{6}d\right)\left(\frac{\epsilon^2}{4}d\right)\right\}\rho^n + \left\{1 - \left(\frac{1-\epsilon^2}{6}d\right)\right. \\ \left. + \left(\frac{1-\epsilon^2}{6}d\right)\left[\frac{1}{5}\left(1 - \frac{\epsilon^2}{4}\right)d\right]\right\}(\rho^T - \rho^n), \end{aligned} \quad (102)$$

whence

$$\begin{aligned} \rho^{n+1} \equiv \rho^T + \left\{\left(\frac{\epsilon^2}{2} + \frac{1-\epsilon^2}{6}\right)d\right\}\rho^n - \left(\frac{1-\epsilon^2}{6}d\right)\left\{\rho^T + \left(\frac{\epsilon^2}{4}d\right)\rho^n\right\} \\ + \left\{\left(\frac{1-\epsilon^2}{6}d\right)\left[\frac{1}{5}\left(1 - \frac{\epsilon^2}{4}\right)d\right]\right\}(\rho^T - \rho^n) \end{aligned} \quad (103)$$

From our earlier experience, the combination

$$\rho^T + \left(\frac{\epsilon^2}{2} + \frac{1-\epsilon^2}{6}\right)d\rho^n$$

is known to be positive for  $|\epsilon| \leq 1/2$ . The remaining terms are

regarded as antidiffusion. The following scheme is

recommended:

$$\rho_j^T = \rho_j^n - \frac{\epsilon}{2}(\rho_{j+1}^n - \rho_{j-1}^n); \quad (104a)$$

$$\rho_j^{TA} = \rho_j^T - \frac{1}{5}\left(1 - \frac{\epsilon^2}{4}\right)(\rho_{j+1}^T - 2\rho_j^T + \rho_{j-1}^T); \quad (104b)$$

$$\rho_j^{TAD} = \rho_j^{TA} + \frac{1}{5}(1 + \epsilon^2)(\rho_{j+1}^n - 2\rho_j^n + \rho_{j-1}^n); \quad (104c)$$

$$\rho_j^{TD} = \rho_j^T + \left(\frac{1}{6} + \frac{\epsilon^2}{3}\right)(\rho_{j+1}^n - 2\rho_j^n + \rho_{j-1}^n); \quad (104d)$$

$$\rho_j^{n+1} = \rho_j^{TD} - \left(\frac{1-\epsilon^2}{6}\right)(\rho_{j+1}^{TAD} - 2\rho_j^{TAD} + \rho_{j-1}^{TAD})^*, \quad (104e)$$

where the asterisk of Eq. (104e) means that the antidiffusive fluxes in this step are to be corrected. It is worth noticing that if  $\rho^{TAD}$  is taken as  $\rho^T$ , we obtain a fourth-order diffusion, fourth-order phase algorithm.

If

$$\rho^{TAD} \equiv \rho^T + \frac{\varepsilon^2}{4} d\phi^n,$$

we get a sixth-order diffusion, fourth-order phase, and finally,

$$\rho^{TAD} \equiv \rho^T + \frac{1}{5}(1 + \varepsilon^2)d\phi^n$$

yields a fourth-order diffusion, sixth-order phase error scheme. The amplitude and phase error versus  $\beta$  are shown in Fig. 9.

## VII. PHYSICAL ASPECTS

The conservation of mass, momentum, and energy applied to a system are expressed as

$$\frac{d}{dt} \int_{\Psi^f(t)} \rho(\vec{x}, t) dV = 0 \quad (111)$$

$$\frac{d}{dt} \int_{\Psi^f(t)} \rho(\vec{x}, t) \vec{u}(\vec{x}, t) dV = \int_{\Psi^f(t)} \rho(\vec{x}, t) \vec{f}(\vec{x}, t) dV + \int_{S^f(t)} \vec{T}(\vec{n}, \vec{x}, t) dS \quad (112)$$

and

$$\begin{aligned} \frac{d}{dt} \int_{\Psi^f(t)} \rho(\vec{x}, t) \left\{ e(\vec{x}, t) + \frac{|\vec{u}(\vec{x}, t)|^2}{2} \right\} dV &= \int_{\Psi^f(t)} \rho(\vec{x}, t) \vec{G}(\vec{x}, t) \cdot \vec{u}(\vec{x}, t) dV \\ &+ \int_{S^f(t)} \vec{T}(\vec{n}, \vec{x}, t) \cdot \vec{u}(\vec{x}, t) dS + \int_{S^f(t)} \vec{q} \cdot \vec{n} dS \end{aligned} \quad (113)$$

where  $e$  and  $G$  are the internal energy and body force per unit mass,  $\vec{T}$  is the stress on an element of surface  $dS$  with unit normal  $\vec{n}$ , and  $\vec{q}$  is the flux of energy through the surface, for example, heat flux. The integrations are carried out over  $\Psi^f(t)$ ,  $S^f(t)$ , where the superscript indicates that the control volume moves with the fluid. We notice that all the terms contributing to the balance of any of the conserved quantities are volume or surface integrals.

In the case of an inviscid fluid

$$\vec{T}(\vec{n}, \vec{x}, t) = -p(\vec{x}, t) \vec{n}. \quad (114)$$

The surface integrals  $\int_{S^f} \vec{T} dS$  and  $\int_{S^f} \vec{T} \cdot \vec{u} dS$  reduce then to  $\int_{S^f} p \vec{n} dS$  and  $\int_{S^f} p \vec{u} \cdot \vec{n} dS$

which yield  $\int_{V^f} \text{grad } p dV$  and  $\int_{V^f} \text{div } (p\vec{u}) dV$ , respectively, when we apply the

divergence theorem.

Recalling Reynold's transport theorem

$$\frac{d}{dt} \int_{V^*(t)} \chi(\vec{x}, t) dV = \int_{V^*(t)} \frac{\partial \chi}{\partial t} dV + \int_{S^*(t)} \chi \vec{u}^* \cdot \vec{n} dS \quad (115)$$

where  $V^*(t)$  is a control volume whose surface elements  $dS$  move with arbitrary velocity  $\vec{u}^*$ . Notice that the two integrals on the RHS are over space and therefore depend only on the instantaneous position of the control volume. Consequently, the integration can be carried out over any control volume which happens to coincide with  $V^*$  at this instant, whether it is fixed or moving with another velocity. Denoting the fluid velocity by  $\vec{u}^f$  and the control surface velocity by  $\vec{u}^g$  we get, using Eq. (115)

$$\begin{aligned} \frac{d}{dt} \int_{V^f} \chi dV &= \int_{V^f} \frac{\partial \chi}{\partial t} dV + \int_{S^f} \chi \vec{u}^f \cdot \vec{n} dS \\ \frac{d}{dt} \int_{V^g} \chi dV &= \int_{V^g} \frac{\partial \chi}{\partial t} dV + \int_{S^g} \chi \vec{u}^g \cdot \vec{n} dS \end{aligned} \quad (116)$$

If  $V^g$  coincide with  $V^f$  at time  $t$ , we get

$$\frac{d}{dt} \int_{V^f} \chi dV = \frac{d}{dt} \int_{V^g} \chi dV + \int_{S^g} (\vec{u}^f - \vec{u}^g) \cdot \vec{n} dS \quad (117)$$

When  $G = 0$  and  $q = 0$ , Eqs. (111) through (113) become

$$\frac{d}{dt} \int_{V^g} \rho dV + \int_{S^g} \rho (\vec{u}^f - \vec{u}^g) \cdot \vec{n} dS = 0; \quad (118)$$

$$\frac{d}{dt} \int_{V^g} \rho \vec{u}^f dV + \int_{S^g} \rho \vec{u}^f [(\vec{u}^f - \vec{u}^g) \cdot \vec{n}] dS = - \int_{S^g} p \vec{n} dS; \quad (119)$$

$$\frac{d}{dt} \int_{V^g} \rho \left( e + \frac{|\vec{u}^f|^2}{2} \right) dV + \int_{S^g} \rho \left( e + \frac{|\vec{u}^f|^2}{2} \right) (\vec{u}^f - \vec{u}^g) \cdot \vec{n} dS = - \int_{S^g} p \vec{u}^f \cdot \vec{n} dS. \quad (120)$$

Using the divergence theorem we can get the differential form of the conservation equations. However, it is far more convenient to use the integral form, because a numerical scheme based on the integral form is already conservative, since the fluxes leaving one control volume have to enter an adjacent one, and discontinuities can be propagated in principle without any smoothing, since one can always integrate a profile including a discontinuity, in contrast with differentiation. Consider Fig. 10, representing a uniform fixed one-dimensional grid and a continuous density profile incorporating one discontinuity. If we know the mass in the hatched cell and the velocity at interfaces A and B, Eq. (118) will give us the rate of change of mass within the cell, and hence the mass itself after an infinitesimal time  $\delta t$ . But we have to get the density at A and B and the velocity for the next time step. We must have recourse then to "averaging" procedures to get the density from a known cell mass and "interpolation" procedures to get the values of the interfaces from the cell average values. Through these two procedures, errors are introduced. Finally, we have to use a finite grid in any case.

Equations (118) to (120) can be written in a reduced form as

$$\frac{d}{dt} \int_{V^g} \rho^* dV + \int_{S^g} \rho^* (\vec{u}^f - \vec{u}^g) \cdot \vec{n} dS = - \int_{S^g} T^* dS + \int_{V^g} G^* dV$$

where  $\rho^*$  is a generalized density ( $\rho^*$  denotes  $\rho$ ,  $\rho \vec{u}^f$  and  $E \equiv \rho(e + \frac{|\vec{u}^f|^2}{2})$  in Eqs. (118) to (120), respectively),  $T^*$  is a generalized surface stress ( $T^* = 0$ ,  $p\vec{n}$ ,  $\rho \vec{u}^f \cdot \vec{n}$ ), while  $G^*$  denotes a generalized body force ( $G^* = 0$  in Eqs. (118) to (120)). The two integrals on the RHS are referred to as source terms.

A naive "finite-integral" form solution can be written as

$$\begin{bmatrix} \text{mass within} \\ \text{control volume} \\ \text{at } t + \delta t \end{bmatrix} = \begin{bmatrix} \text{mass within} \\ \text{control volume} \\ \text{at } t \end{bmatrix} - \begin{bmatrix} \text{net outgoing} \\ \text{mass flux through} \\ \text{control surface} \end{bmatrix} + [\text{source terms}].$$

As will be explained next, the above formula is supplemented with diffusion flux terms (actually diffusion and antidiffusion) to improve its accuracy.

## ACCURACY

The above mathematical analysis was carried out assuming a fixed uniform grid and  $\frac{\partial \rho}{\partial t} + u_0 \frac{\partial \rho}{\partial x} = 0$ , where  $u_0 \equiv \text{constant}$ . We notice also the absence of any source term (inhomogeneous part of a conservation equation). The analytical solution was found out to be

$$\rho^{n+1} = A \rho^n$$

where  $A = e^{-i\beta c}$ , then was expanded to get a numerical scheme that matches it up to a prescribed order of  $\beta$ . In this context the numerical scheme

is an approximate solution of the whole PDE, in contrast to schemes which approximate  $\frac{\partial}{\partial x}$  alone by a finite difference and  $\frac{\partial}{\partial t}$  alone. By getting a solution of the PDE as a whole, we mix the time and space derivatives for a higher order scheme. To see that, let us expand  $\rho(t + \delta t, x)$  in a Taylor series:

$$\rho(t + \delta t, x) = \rho(t) + \delta t \left. \frac{\partial \rho}{\partial t} \right|_x + \frac{\delta t^2}{2!} \left. \frac{\partial^2 \rho}{\partial t^2} \right|_x + \dots \quad (121)$$

From the PDE

$$\frac{\partial \rho}{\partial t} = -u_0 \frac{\partial \rho}{\partial x} \quad (122a)$$

$$\frac{\partial^2 \rho}{\partial t^2} = \frac{\partial}{\partial t} \left( \frac{\partial \rho}{\partial t} \right) = \frac{\partial}{\partial t} \left( -u_0 \frac{\partial \rho}{\partial x} \right) = -u_0 \frac{\partial}{\partial x} \left( \frac{\partial \rho}{\partial t} \right) - u_0^2 \frac{\partial^2 \rho}{\partial x^2} \quad (122b)$$

Substituting Eqs. (122) into (121) we obtain

$$\rho(t + \delta t, x) = \rho(t) - u_0 \delta t \frac{\partial \rho}{\partial x} + \frac{u_0^2 \delta t^2}{2} \frac{\partial^2 \rho}{\partial x^2} + \dots, \quad (123)$$

showing that we can get a better solution in the time domain (of higher order in  $\delta t$ ) by adding to  $[\rho(t) - u_0 \delta t \frac{\partial \rho}{\partial x}]$  a diffusion term,

$\frac{u_0^2 \delta t^2}{2} \frac{\partial^2 \rho}{\partial x^2}$ , a purely spatial derivative. Notice that  $\frac{u_0^2 (\delta t)^2}{2}$  is equivalent to  $\frac{\epsilon^2}{2}$ , the coefficient of  $d\rho^n$  in the schemes discussed earlier. The remaining terms appear when we try to express  $\frac{\partial \rho}{\partial x}$  and  $\frac{\partial^2 \rho}{\partial x^2}$  in terms of finite differences accurately.

A scheme which splits the time and space domains, on the other hand, treats Eq. (122a) as an ODE, where the right-hand side is assumed to be a function of time. A second-order Runge-Kutta explicit scheme can be written as



$$\rho(t + \delta t, x) = \rho(t, x) - u_0 \delta t \frac{\partial \rho}{\partial x} \Big|_{t + \frac{\delta t}{2}, x} \quad (124)$$

where  $\frac{\partial \rho}{\partial x} \Big|_{t + \frac{\delta t}{2}, x}$  is obtained by first getting a provisional value of the density at  $t + \delta t/2$  using a lower-order scheme

$$\rho(t + \frac{\delta t}{2}, x) = \rho(t, x) - u_0 \frac{\delta t}{2} \frac{\partial \rho}{\partial x} \Big|_{t, x} \quad (125)$$

then getting  $\frac{\partial \rho}{\partial x} \Big|_{t + \frac{\delta t}{2}, x}$  by differentiating  $\rho(t + \frac{\delta t}{2}, x)$  spatially, with the result

$$\frac{\partial \rho}{\partial x} \Big|_{t + \frac{\delta t}{2}, x} = \frac{\partial \rho}{\partial x} \Big|_{t, x} - u_0 \frac{\delta t}{2} \frac{\partial^2 \rho}{\partial x^2} \Big|_{t, x}.$$

Upon substituting in Eq. (124), this yields Eq. (123) again. One can deduce therefore that up to a given order, schemes which mix the time and space domains and those which split them are equivalent. A warning, however, is in order here: A concept derived for a split time-space scheme cannot be applied directly to one that mixes both domains. For example, using a half point density in Eq. (123), i.e., the scheme

$$\rho(t + \frac{\delta t}{2}, x) = \rho(t, x) - u_0 \frac{\delta t}{2} \frac{\partial \rho}{\partial x} \Big|_{t, x} + \frac{u_0^2 \delta t^2}{8} \frac{\partial^2 \rho}{\partial x^2} \Big|_{t, x} \quad (126a)$$

$$\rho(t + \delta t, x) = \rho(t, x) - u_0 \delta t \frac{\partial \rho}{\partial x} \Big|_{t + \frac{\delta t}{2}, x} + \frac{u_0^2 \delta t^2}{2} \frac{\partial^2 \rho}{\partial x^2} \Big|_{t + \frac{\delta t}{2}, x} \quad (126b)$$

will cause a decrease in accuracy instead of improving it, as can be seen from differentiating Eq. (126a) with respect to  $x$  and substituting in Eq. (126b). The key point is that Eq. (123) is a solution of the PDE as a whole.

In summary, the schemes derived in earlier sections are solutions of the conservation equations if  $u^f = \text{constant}$ ,  $u^g = 0$ , and source terms = 0.

If these are not satisfied, a correction that preserves the order of the scheme should be adopted. Here we split the two effects:

(1)  $u^f$  variable and source terms are variable  $\neq 0$

(2)  $u^g \neq 0$

and treat each separately.

### GRID MOTION

According to the above splitting, we need to consider a case where  $u^f = 0$  and source terms vanish, but  $u^g \neq 0$ . This is a static field, where the density and energy are constants. Equations (118) and (120) reduce then to

$$\frac{d}{dt} \int_{V^g} dV = \int_{S^g} \vec{u}^g \cdot \vec{n} dS \quad (127)$$

This exhibits the formula for an accurate scheme when the grid is moving: the rate of change of volume equals the rate of sweeping by the moving surface, as illustrated in Fig. 11. Here we can achieve an infinite-order accuracy in  $\delta t$  by defining a mean control area  $S^{\text{mean}}$  such that

$$\int_{S^{\text{mean}}} \vec{u}^g \delta t \cdot \vec{n} dS = \text{swept volume}$$

Let us consider the three cases of 1-D geometry; namely, planar, cylindrical, and spherical symmetries, denoted from now on by  $\chi = 1, 2$ , and 3, respectively.

In the planar case, the area is independent of the radius, so that

$$A_L^{n+\frac{1}{2}} = A_R^{n+\frac{1}{2}} = 1, \quad (128)$$

where L and R denote the left and right interfaces of the control cell, respectively.

In cylindrical 1-D geometry, the volume swept by the interface is

$$\Delta \Psi_B = \pi[(r_B^{n+1})^2 - (r_B^n)^2],$$

where B indicates L or R. Here the depth of the cell being considered is taken equal to unity. Since  $u^g \delta t = r_B^{n+1} - r_B^n$ , the average area is

$$A_B^{n+\frac{1}{2}} \equiv \frac{\Delta \Psi_B}{u^g \delta t} = \pi \frac{[(r_B^{n+1})^2 - (r_B^n)^2]}{r_B^{n+1} - r_B^n} = \pi(r_B^{n+1} + r_B^n) \quad (129)$$

One can define then average radii

$$r_B^{n+\frac{1}{2}} \equiv \frac{1}{2}(r_B^n + r_B^{n+1}), \quad (130)$$

since  $A_B^{n,n+\frac{1}{2},n+1} = 2\pi r_B^{n,n+\frac{1}{2},n+1}$ .

Finally, in spherical geometry, the swept volume is

$$\Delta \Psi = \frac{4}{3} \pi[(r_B^{n+1})^3 - (r_B^n)^3],$$

yielding

$$A_B^{n+\frac{1}{2}} \equiv \frac{\Delta \Psi}{r_B^{n+1} - r_B^n} = \frac{4}{3} \pi[(r_B^n)^2 + (r_B^n)(r_B^{n+1}) + (r_B^{n+1})^2]. \quad (131)$$

whence

$$r_B^{n+\frac{1}{2}} = \left\{ \frac{1}{3}[(r_B^n)^2 + (r_B^n)(r_B^{n+1}) + (r_B^{n+1})^2] \right\}^{\frac{1}{2}}, \quad (132)$$

since

$$A_B^{n,n+\frac{1}{2},n+\frac{1}{2}} = 4\pi(r_B^{n,n+\frac{1}{2},n+1})^2.$$

Equations (128), (129), and (131) should be used as the proper interface areas when evaluating the fluxes and surface forces. To complete the formulation, when body forces are present, the volume used should be that confined between the average interfaces. It can be arbitrarily selected for  $\alpha = 1$ , and is defined as

$$V^{n+\frac{1}{2}} = \pi[(r_R^{n+\frac{1}{2}})^2 - (r_L^{n+\frac{1}{2}})^2] \quad (133)$$

for  $\alpha = 2$ , and

$$V^{n+\frac{1}{2}} = \frac{4}{3} \pi[(r_R^{n+\frac{1}{2}})^3 - (r_L^{n+\frac{1}{2}})^3] \quad (134)$$

for  $\alpha = 3$ . This choice will ensure a proper balance between surface and body forces.

### Variable Velocity Field and Source Terms

To account for these two effects, the fluid velocity and source terms used in the "finite-integral" solution should be evaluated at some intermediate time between  $t^n$ ,  $t^{n+1}$  so as to preserve the accuracy of the scheme. Since we split the effects of grid motion, variable velocity field and source terms, the above intermediate values should be derived from an ODE solver of a consistent order in  $\delta t$ . For a fourth-order (diffusion and phase error) accurate scheme, for example, we need a second-order-accurate explicit ODE solver. In other words, for the system of Eqs. (118) to (120), we advance the time one-half step using  $\vec{u}^f = \vec{u}^n$  and  $p = p^n$  to get  $\rho^{n+\frac{1}{2}}$ ,  $(\rho \vec{u}^f)^{n+\frac{1}{2}}$ ,  $E^{n+\frac{1}{2}}$ . We define  $\vec{u}^{n+\frac{1}{2}} \equiv (\rho \vec{u}^f)^{n+\frac{1}{2}} / \rho^{n+\frac{1}{2}}$  and  $p^{n+\frac{1}{2}} \equiv p(\rho^{n+\frac{1}{2}}, e^{n+\frac{1}{2}})$  where  $p(\rho, e)$  is the equation of state and

$$e^{n+1/2} = (E^{n+1/2} / \rho^{n+1/2}) - \frac{|\vec{u}^{n+1/2}|^2}{2}.$$

Then we advance the system a whole time step using  $\vec{u}^f = \vec{u}^{n+1/2}$  and  $p = p^{n+1/2}$ . As explained earlier, we need not and should not update  $\rho$ ,  $\rho \vec{u}^f$  and  $E$ , during the full time step, since the scheme is already a solution of the whole PDE. For a sixth-order-accurate scheme, we need a fourth-order ODE solver and so on.

### Example of an Algorithm

Let us implement the scheme

$$\rho_j^T = \rho_j^n - \frac{\varepsilon}{2}(\rho_{j+1}^n - \rho_{j-1}^n) + \frac{\varepsilon^2}{4}(\rho_{j+1}^n - 2\rho_j^n + \rho_{j-1}^n);$$

$$\rho_j^{TD} = \rho_j^T + \left(\frac{1}{6} + \frac{\varepsilon^2}{12}\right)(\rho_{j+1}^n - 2\rho_j^n + \rho_{j-1}^n);$$

$$\rho_j^{n+1} = \rho_j^{TD} - \left(\frac{1}{6} - \frac{\varepsilon^2}{6}\right)(\rho_{j+1}^T - 2\rho_j^T + \rho_{j-1}^T), \quad (135)$$

a stable, fourth-order phase error, sixth-order diffusion error scheme,

where  $\rho$  denotes either of  $\rho$ ,  $\rho \vec{u}^f$ , or  $E$ .

If we have  $N$  cells whose interfaces are at radii  $(r_{1/2}^n, r_{3/2}^n, \dots, r_{N+1/2}^n)$  at time  $t^n$ , moving to  $(r_{1/2}^{n+1}, r_{3/2}^{n+1}, \dots)$  at  $t^{n+1}$ , let us denote the cell centers by the subscripts  $j = 1, 2, \dots, N$ , located at

$$r_j^{n,n+1} \equiv \begin{cases} \frac{1}{2}(r_{j-1/2}^{n,n+1} + r_{j+1/2}^{n,n+1}) & \text{for } \alpha = 1, 2 \\ \left\{ \frac{1}{3}[(r_{j-1/2}^{n,n+1})^2 + (r_{j-1/2}^{n,n+1})(r_{j+1/2}^{n,n+1}) + (r_{j+1/2}^{n,n+1})^2] \right\}^{1/2} & \text{for } \alpha = 3. \end{cases} \quad (136)$$

The volume of the  $j^{\text{th}}$  cell per unit angle is given by

$$\psi_j^{n,n+1} = \begin{cases} r_{j+1/2}^{n,n+1} - r_{j-1/2}^{n,n+1}, & \alpha = 1 \\ \frac{1}{2} [(r_{j+1/2}^{n,n+1})^2 - (r_{j-1/2}^{n,n+1})^2], & \alpha = 2 \\ \frac{1}{3} [(r_{j+1/2}^{n,n+1})^3 - (r_{j-1/2}^{n,n+1})^3], & \alpha = 3 \end{cases} \quad (137)$$

Denoting the mean interface radii by  $r_{j+\frac{1}{2}}^{n+\frac{1}{2}}$ , Eqs. (128), (130), and (132) imply for  $j = 0, \dots, N$ ,

$$r_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \begin{cases} (r_{j+\frac{1}{2}}^n + r_{j+\frac{1}{2}}^{n+1})/2 & \alpha = 1, 2 \\ \left[ \frac{(r_{j+\frac{1}{2}}^n)^2 + (r_{j+\frac{1}{2}}^n)(r_{j+\frac{1}{2}}^{n+1}) - (r_{j+\frac{1}{2}}^{n+1})^2}{3} \right]^{\frac{1}{2}}, & \alpha = 3 \end{cases} \quad (138)$$

giving, according to Eqs. (128), (129), and (131), mean interface area per unit angle

$$A_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \begin{cases} 1 \\ r_{j+\frac{1}{2}}^{n+\frac{1}{2}} \\ (r_{j+\frac{1}{2}}^{n+\frac{1}{2}})^2 \end{cases} \quad (139)$$

and mean cell volume per unit angle

$$\psi_j^{n+\frac{1}{2}} = \begin{cases} (r_{j+\frac{1}{2}}^{n+\frac{1}{2}} - r_{j-\frac{1}{2}}^{n+\frac{1}{2}}) \\ \frac{1}{2} [(r_{j+\frac{1}{2}}^{n+\frac{1}{2}})^2 - (r_{j-\frac{1}{2}}^{n+\frac{1}{2}})^2] \\ \frac{1}{3} [(r_{j+\frac{1}{2}}^{n+\frac{1}{2}})^3 - (r_{j-\frac{1}{2}}^{n+\frac{1}{2}})^3] \end{cases} \quad (140)$$

for  $\alpha = 1, 2, 3$ , respectively. We write Eq. (135a) in the form

$$\begin{aligned}
\psi_j^{n+1} T_j = \psi_j^n \rho_j^n - \delta t (\rho_{j+\frac{1}{2}}^n A_{j+\frac{1}{2}}^{n+\frac{1}{2}} \delta U_{j+\frac{1}{2}}^{n+\frac{1}{2}}) + \delta t (\rho_{j-\frac{1}{2}}^n A_{j-\frac{1}{2}}^{n+\frac{1}{2}} \delta U_{j-\frac{1}{2}}^{n+\frac{1}{2}}) \\
+ \lambda_{j+\frac{1}{2}}^{n+\frac{1}{2}} \psi_{j+\frac{1}{2}}^n (\rho_{j+\frac{1}{2}}^n - \rho_j^n) - \lambda_{j-\frac{1}{2}}^{n+\frac{1}{2}} \psi_{j-\frac{1}{2}}^n (\rho_j^n - \rho_{j-1}^n) + \text{source}_j^{n+\frac{1}{2}},
\end{aligned} \quad (141)$$

where

$$\rho_{j+\frac{1}{2}}^n = \frac{1}{2}(\rho_j^n + \rho_{j+1}^n) \quad (142)$$

for  $j = 1, \dots, N-1$ , while

$$\rho_{\frac{1}{2}}^n = \frac{1}{2}(\rho_L^n + \rho_1^n), \quad \rho_{N-\frac{1}{2}}^n = \frac{1}{2}(\rho_N^n + \rho_R^n),$$

where L and R denote left and right guard cells, respectively. The difference  $\delta U_{j+\frac{1}{2}}$  between the fluid and grid velocities is given by

$$\delta U_{j+\frac{1}{2}}^{n+\frac{1}{2}} \delta t = U_{j+\frac{1}{2}}^{n+\frac{1}{2}} \delta t - U_{j+\frac{1}{2}}^g \delta t = U_{j+\frac{1}{2}}^{n+\frac{1}{2}} \delta t - (r_{j+\frac{1}{2}}^{n+1} - r_{j+\frac{1}{2}}^n), \quad (143)$$

while the diffusion coefficient is

$$\lambda_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{1}{4}(\epsilon_{j+\frac{1}{2}}^{n+\frac{1}{2}})^2, \quad (144)$$

where

$$\epsilon_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{\delta U_{j+\frac{1}{2}}^{n+\frac{1}{2}} A_{j+\frac{1}{2}}^{n+\frac{1}{2}} \delta t}{2} \left( \frac{1}{\psi_j^n} + \frac{1}{\psi_{j+1}^n} \right). \quad (145)$$

The velocity at the interfaces satisfies

$$U_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{1}{2}(U_j^{n+\frac{1}{2}} + U_{j+1}^{n+\frac{1}{2}}) \quad (146)$$

for  $j = 1, \dots, N-1$ , while

$$U_{j+\frac{1}{2}}^{n+\frac{1}{2}} = U_L^{n+\frac{1}{2}}, U_{N+\frac{1}{2}}^{n+\frac{1}{2}} = U_R^{n+\frac{1}{2}}.$$

The volumes  $\Psi_{j+\frac{1}{2}}^n$  are defined as

$$\Psi_{j+\frac{1}{2}}^n = \frac{1}{2}(\Psi_j^n + \Psi_{j+1}^n) \quad (147)$$

for  $j = 1, \dots, N-1$ , and

$$\Psi_{\frac{1}{2}}^n = \Psi_1^n, \Psi_{N+\frac{1}{2}}^n = \Psi_N^n.$$

Equation (135b) then adds the main diffusion, giving

$$\Psi_j^{n+1} \rho_j^{TD} = \Psi_j^{n+1} \rho_j^T + v_{j+\frac{1}{2}}^{n+\frac{1}{2}} \Psi_{j+\frac{1}{2}}^n (\rho_{j+1}^n - \rho_j^n) - v_{j-\frac{1}{2}}^{n+\frac{1}{2}} \Psi_{j-\frac{1}{2}}^n (\rho_j^n - \rho_{j-1}^n) \quad (148)$$

where

$$v_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{1}{6} + \frac{(\varepsilon_{j+\frac{1}{2}}^{n+\frac{1}{2}})^2}{12}. \quad (149)$$

Finally, the antidiffusive fluxes are evaluated according to

$$F_{j+\frac{1}{2}} = u_{j+\frac{1}{2}}^{n+\frac{1}{2}} \Psi_{j+\frac{1}{2}}^{n+1} (\rho_{j+1}^T - \rho_j^T), \quad (150)$$

where

$$u_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{1}{6} - \frac{(\varepsilon_{j+\frac{1}{2}}^{n+\frac{1}{2}})^2}{6}, \quad (151)$$

and then corrected using one of the flux limiters Eq. (64) or Eqs. (65)-(75).

Let us select Eq. (64) on account of its simplicity. The corrected fluxes are given by

$$F_{j+\frac{1}{2}}^C = \text{sign}(F_{j+\frac{1}{2}}) \cdot \max \{0, \min [\text{sign}(F_{j+\frac{1}{2}}) \cdot \Psi_{j+\frac{1}{2}}^{n+1} \cdot (\rho_{j+2}^{TD} - \rho_{j+1}^{TD}), |F_{j+\frac{1}{2}}|, \text{sign}(F_{j+\frac{1}{2}}) \cdot \Psi_{j-\frac{1}{2}}^{n+1} \cdot (\rho_j^{TD} - \rho_{j-1}^{TD})]\} \quad (152)$$

whence



$$\phi_j^{n+1} = \phi_j^{TD} - \frac{1}{v_j^{n+1}} (F_{j+\frac{1}{2}}^C - F_{j-\frac{1}{2}}^C). \quad (153)$$

As for the source terms, they are summations over the surface or the volume of the cell. Let us consider first  $[-\int_{S^g} p n dS]$ , which yields  $[-\text{grad } p]$ . In cartesian coordinates, following the diagram of Fig. 12,

$$\text{source } \frac{n+1}{j} = p_{j-\frac{1}{2}}^{n+1} A_{j-\frac{1}{2}}^{n+1} - p_{j+\frac{1}{2}}^{n+1} A_{j+\frac{1}{2}}^{n+1} \quad (154)$$

where

$$p_{j+\frac{1}{2}}^{n+1} = \frac{1}{2}(p_j^{n+1} + p_{j+1}^{n+1}) \quad (155)$$

for  $j = 1, \dots, N-1$ , while  $p_{\frac{1}{2}}^{n+1} = p_L^{n+1}$  and  $p_{N+\frac{1}{2}}^{n+1} = p_R^{n+1}$ .

In cylindrical geometry, following Fig. 13, we have

$$\text{source } \frac{n+1}{j} = p_{j-\frac{1}{2}}^{n+1} A_{j-\frac{1}{2}}^{n+1} - p_{j+\frac{1}{2}}^{n+1} A_{j+\frac{1}{2}}^{n+1} + p_j^{n+1} (r_{j+\frac{1}{2}}^{n+1} - r_{j-\frac{1}{2}}^{n+1})$$

and since

$$r_{j+\frac{1}{2}}^{n+1} - r_{j-\frac{1}{2}}^{n+1} = \frac{(r_{j+\frac{1}{2}}^{n+1})^2 - (r_{j-\frac{1}{2}}^{n+1})^2}{r_{j+\frac{1}{2}}^{n+1} + r_{j-\frac{1}{2}}^{n+1}} = \frac{v_j^{n+1}}{r_j^{n+1}},$$

where from Eq. (136)

$$r_j^{n+1} = \frac{1}{2}(r_{j+\frac{1}{2}}^{n+1} + r_{j-\frac{1}{2}}^{n+1}) \quad (156)$$

for  $\alpha = 2$ , we can rewrite the expression for source  $\frac{n+1}{j}$  as

$$\text{source } \frac{n+1}{j} = p_{j-\frac{1}{2}}^{n+1} A_{j-\frac{1}{2}}^{n+1} - p_{j+\frac{1}{2}}^{n+1} A_{j+\frac{1}{2}}^{n+1} + \frac{p_j^{n+1}}{r_j^{n+1}} v_j^{n+1}, \quad (157)$$

where we notice that  $p_j^{n+1}/r_j^{n+1}$  acts as a body force per unit volume per unit angle.

In spherical geometry,

$$\begin{aligned} \text{source } j^{n+1} &= p_{j-\frac{1}{2}}^{n+1} A_{j-\frac{1}{2}}^{n+1} - p_{j+\frac{1}{2}}^{n+1} A_{j+\frac{1}{2}}^{n+1} + p_j^{n+1} [(r_{j+\frac{1}{2}}^{n+1})^2 \\ &\quad - (r_{j-\frac{1}{2}}^{n+1})^2] = p_{j-\frac{1}{2}}^{n+1} A_{j-\frac{1}{2}}^{n+1} - p_{j+\frac{1}{2}}^{n+1} A_{j+\frac{1}{2}}^{n+1} \\ &\quad + \frac{2p_j^{n+1}}{(r_j^{n+1})^2/r_{j,\alpha=2}^{n+1}} v_j^{n+1}, \end{aligned}$$

where from Eq. (136),

$$r_j^{n+1} = \frac{1}{3} [(r_{j-\frac{1}{2}}^{n+1})^2 + (r_{j+\frac{1}{2}}^{n+1})(r_{j-\frac{1}{2}}^{n+1}) + (r_{j+\frac{1}{2}}^{n+1})^2] \quad (159)$$

for  $\alpha = 3$ , and

$$r_{j,\alpha=2}^{n+1} = \frac{r_{j+\frac{1}{2}}^{n+1} + r_{j-\frac{1}{2}}^{n+1}}{2}$$

Again,  $\frac{2p_j^{n+1}}{(r_j^{n+1})^2/r_{j,\alpha=2}^{n+1}}$  acts as a body force per unit volume per unit angle.

Next we consider  $[-\int_{S^g} \vec{p} \cdot \vec{n} dS]$ , which gives rise to the term  $[-\text{div}(\vec{p})]$ .

For the three geometries, we get

$$\text{source } j^{n+1} = p_{j-\frac{1}{2}}^{n+1} U_{j-\frac{1}{2}}^{n+1} A_{j-\frac{1}{2}}^{n+1} - p_{j+\frac{1}{2}}^{n+1} U_{j+\frac{1}{2}}^{n+1} A_{j+\frac{1}{2}}^{n+1} \quad (160)$$

In summary, all we need for the source terms is a routine to multiply by the frontal area for the surface integrals, or cell volume in the case volume integrals.

Finally,  $U_j^{n+1/2}$  and source  $j^{n+1/2}$  are obtained by first advancing the whole system of Eqs. (136)-(160) a half time step using  $U_j^n$ , source  $j^n$ , then a whole time step using

$$U_j^{n+1/2}|_{t \rightarrow t+\delta t} = U_j^{n+1}|_{t \rightarrow t+\delta t/2} \quad (161)$$

and

$$\text{source } j^{n+1/2}|_{t \rightarrow t+\delta t} = \text{source } j^{n+1}|_{t \rightarrow t+\delta t/2}. \quad (162)$$

# XI. TWO-DIMENSIONAL TRANSPORT

Now let us consider the two-dimensional equivalent of Eq. (2),

$$\frac{\partial \rho}{\partial t} + u_1 \frac{\partial \rho}{\partial x} + u_2 \frac{\partial \rho}{\partial y} = 0, \quad (201)$$

whose analytic solution is

$$\rho(x, y, t) = \rho(x - u_1 t, y - u_2 t, 0), \quad (202)$$

a wave propagating with velocity  $\vec{u} = (u_1, u_2)$ . Assuming an initial density  $\rho(x, y, 0) = F(x, y)$ , we Fourier analyze  $F(x, y)$  in space on a rectangle  $L_1 \times L_2$  with periodic boundary conditions:

$$F(\vec{r}) = \sum_{\vec{k}=-\infty}^{\infty} \hat{\rho}_{\vec{k}} e^{-i\vec{k} \cdot \vec{r}}, \quad (203a)$$

where  $\vec{r} = (x, y)$ , and  $\vec{k} = (k_1, k_2)$  is assumed to be normalized, i.e.,  $\vec{k}$  denotes  $2\pi(\frac{k_1}{L_1}, \frac{k_2}{L_2})$ . Notice that the summation of (203a) is actually a double summation.

$$F(x, y) = \sum_{k_1=-\infty}^{\infty} \sum_{k_2=-\infty}^{\infty} \hat{\rho}_{k_1, k_2} e^{i(k_1 x + k_2 y)}. \quad (203b)$$

To gain insight, let us consider only one wave component of Eq.

(203),

$$F(\vec{r}) = \sin \vec{k} \cdot \vec{r} \quad (204a)$$

or

$$F(x, y) = \sin 2\pi \left( \frac{k_1 x}{L_1} + \frac{k_2 y}{L_2} \right). \quad (204b)$$

Figure 21 shows the resulting waves for different values of  $(L_1, L_2)$ ,  $(k_1, k_2)$ .

From Eq. (204b),  $F(x, y)$  is constant along lines of constant

$(\frac{k_1 x}{L_1} + \frac{k_2 y}{L_2})$ . For example, the nodes of the wave coincide with the lines

$$\frac{k_1 x}{L_1} + \frac{k_2 y}{L_2} = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \dots \quad (205)$$

which are normal to the wave vector  $\vec{k}$ .

To find the wave length for a given  $(k_1, k_2)$ , we first go back to the one-dimensional case. For a system of length  $L$  and periodic boundary conditions, the harmonics  $\sin 2\pi \frac{kx}{L}$  and  $\cos 2\pi \frac{ky}{L}$  are admitted, where  $k = 0, 1, 2, \dots, \infty$ . With each of these is associated a wave length  $\lambda$  defined as the distance between two successive "even" nodes. Since  $\sin 2\pi \frac{kx}{L} = 0$  at  $\frac{2\pi kx}{L} = 0, \pi, 2\pi, 3\pi, \dots$ ,  $\lambda$  is obtained from  $\frac{2\pi k\lambda}{L} = 2\pi$ , yielding

$$\lambda = \frac{L}{k}. \quad (206)$$

We get therefore wave lengths  $\infty, L, \frac{L}{2}, \frac{L}{3}, \frac{L}{4}, \dots$ , where the longest finite wave length equals  $L$ , the system length. In two-dimensional, the wave length for a given  $k$  is defined analogously as the distance between two points on successive "even" node lines, projected on the direction of  $\vec{k}$ .

From Eq. (204b),

$$F(x, 0) = \sin 2\pi \frac{k_1 x}{L_1}$$

which, as explained above, yields  $\lambda_x = \frac{L_1}{k_1}$  where  $\lambda_x$  is the wave length along the  $x$ -direction, which when projected on  $k = 2\pi(\frac{k_1}{L_1}, \frac{k_2}{L_2})$  yields  $\lambda$ :

$$\lambda = \frac{(\frac{L_1}{k_1}, 0) \cdot (\frac{k_1}{L_1}, \frac{k_2}{L_2})}{\sqrt{(\frac{k_1}{L_1})^2 + (\frac{k_2}{L_2})^2}} = \frac{1}{\sqrt{(\frac{k_1}{L_1})^2 + (\frac{k_2}{L_2})^2}} = \frac{2\pi}{|\vec{k}|}, \quad (207a)$$

where

$$|\vec{k}| = \sqrt{\left(\frac{2\pi k_1}{L_1}\right)^2 + \left(\frac{2\pi k_2}{L_2}\right)^2}$$

or

$$\lambda = \frac{1}{\sqrt{\left(\frac{1}{\lambda_x}\right)^2 + \left(\frac{1}{\lambda_y}\right)^2}} \quad (207b)$$

Now we find all the wavelengths along a given direction  $\frac{k_1}{L_1} : \frac{k_2}{L_2} =$  constant  $c$ . Noticing that  $k_1, k_2$  for periodic boundary conditions can take only integer values, the waves along a given direction correspond to

$k_1^{(n)} = nk_1^{(1)}, k_2^{(n)} = nk_2^{(1)}$  ( $n = 1, 2, \dots, \infty$ ) where  $k_1^{(1)}, k_2^{(1)}$  are the smallest integers that satisfy

$$\frac{k_1^{(1)}/L_1}{k_2^{(1)}/L_2} = c$$

From Eq. (207a)

$$\lambda_n = \frac{1}{\sqrt{\frac{nk_1^{(1)}}{L_1}^2 + \frac{nk_2^{(1)}}{L_2}^2}} = \frac{\lambda_1}{n}, \quad (208)$$

where

$$\lambda_1 = \frac{1}{\sqrt{\frac{k_1^{(1)}}{L_1}^2 + \frac{k_2^{(1)}}{L_2}^2}}. \quad (209)$$

Along a given direction we have wave lengths  $\lambda_1, \frac{\lambda_1}{2}, \frac{\lambda_1}{3}, \dots, \frac{\lambda_1}{\infty}$ .

Consider, for example, Fig. 21(b), where  $L_1 = 2, L_2 = 1$ . Along direction

$(1/2, 1)$ ,  $k_1^{(1)} = k_2^{(1)} = 1$ , whence  $\lambda_1 = 1/\sqrt{(\frac{1}{2})^2 + 1} = 2/\sqrt{5}$ . The maximum system length along this direction being  $\sqrt{(\frac{1}{2})^2 + 1} = \frac{\sqrt{5}}{2}$ ,  $\frac{\lambda_1}{L_{1,1}} = \frac{2/\sqrt{5}}{\sqrt{5}/2} = \frac{4}{5}$ , showing that because of the periodic boundary condition independently in each direction the longest wave length is only 80 percent of the maximum system length in the direction  $(\frac{1}{2}, 1)$ , in contrast to one-dimensional cases where  $\lambda_1 = L$ . For the case of Fig. 21(a),  $\lambda_1$  is 50 percent of the system length.

From Eq. (202),

$$\begin{aligned} \rho(x, y, t) &= \sum_{k_1=-\infty}^{\infty} \sum_{k_2=-\infty}^{\infty} \hat{\rho}_{k_1, k_2} e^{i[k_1(x - u_1 t) + k_2(y - u_2 t)]} \\ &= \sum_{k_1} \sum_{k_2} \hat{\rho}_{k_1, k_2}(t) e^{i(k_1 x + k_2 y)} \end{aligned} \quad (210a)$$

or

$$\rho(\vec{r}, t) = \sum_{\vec{k}=-\infty}^{\infty} \hat{\rho}_{\vec{k}} e^{i\vec{k} \cdot (\vec{r} - \vec{u}t)} = \sum_{\vec{k}} \hat{\rho}_{\vec{k}} e^{i\vec{k} \cdot \vec{r}} \quad (210b)$$

where

$$\hat{\rho}_{k_1, k_2}(t) = \hat{\rho}_{k_1, k_2} e^{-i(k_1 u_1 + k_2 u_2)t} \quad (211a)$$

or

$$\hat{\rho}_{\vec{k}}(t) = \hat{\rho}_{\vec{k}} e^{-i\vec{k} \cdot \vec{u}t} \quad (211b)$$

Thus each harmonic independently advances uniformly in phase without changing its magnitude, as shown in Fig. (22).

We notice that the different harmonics advance in the direction  $\vec{u}$ , which is generally different from that of  $\vec{k}$ , as illustrated in Fig. (23). They keep their front normal to  $\vec{k}$  and therefore the projection of  $\vec{u}$  on  $\vec{k}$  is the speed of advance. This adds extra requirements that were not invoked in the one-dimensional case, namely:

1. The scheme should keep the wave front a straight line; otherwise distortion of profiles occurs.
2. It should also keep the wave front normal to  $\vec{k}$ ; otherwise "scattering" occurs, namely waves with different  $|\vec{k}|$  but the same direction  $(k_1:k_2)$  will come out in different directions, causing scattering of the transported profile.

As will be proved later, the speed of propagation  $\vec{V}$  of a numerical scheme differs from  $\vec{u}$  not only in magnitude as in one dimension but also in direction, providing one more source of error. If the above two requirements are satisfied, however, only  $\vec{k} \cdot (\vec{V} - \vec{u})$  contributes to the phase error.

Now suppose  $\phi$  is known at all times only on a set of  $(N_1 + 1) \cdot (N_2 + 1)$  discrete grid points with separation  $\delta x = \frac{L_1}{N_1}$ ,  $\delta y = \frac{L_2}{N_2}$ , namely,  $x_i = i\delta x$  ( $i = 0, 1, \dots, N_1 - 1$ ),  $y_j = j\delta y$  ( $j = 0, 1, \dots, N_2 - 1$ ), the origin being a member of the set. According to periodicity assumption  $\phi_{0,j} = \phi_{N_1,j}$ ,  $\phi_{i,0} = \phi_{i,N_2}$ ; hence we can have only  $\frac{N_1 N_2}{2} + 1$  different harmonics. Let

$$f(x, y) = \sum_{k_1 = -\frac{N_1}{2}}^{\frac{N_1}{2}} \sum_{k_2 = -\frac{N_2}{2}}^{\frac{N_2}{2}} \hat{\phi}_{k_1, k_2} e^{i(k_1 x + k_2 y)}. \quad (212)$$



Since

$$\begin{aligned}
 e^{i(k_1 x + k_2 y)} \Big|_{k_1 = \frac{N_1}{2}} &= e^{i\left(\frac{2\pi}{L_1}\left(\frac{N_1}{2}\right)\delta x + \frac{2\pi k_2}{L_2} j\delta y\right)} = e^{i\left(i\pi + 2\pi \frac{k_2}{L_2} j\delta y\right)} \\
 &= e^{i\left[i\pi + 2\pi \frac{k_2}{L_2} j\delta y\right] - 2\pi i} = e^{i\left(-i\pi + \frac{2\pi k_2}{L_2} j\delta y\right)} \\
 &= e^{i\left[\frac{2\pi}{L_1}\left(-\frac{N_1}{2}\right)\delta x + \frac{2\pi k_2}{L_2} j\delta y\right]} = e^{i(k_1 x + k_2 y)} \Big|_{k_1 = -\frac{N_1}{2}}
 \end{aligned}$$

for all  $i$ , and similarly

$$e^{i(k_1 x + k_2 y)} \Big|_{k_2 = \frac{N_2}{2}} = e^{i(k_1 x + k_2 y)} \Big|_{k_2 = -\frac{N_2}{2}}$$

for all  $j$ , Eq. (212) can be rewritten as

$$\begin{aligned}
 f(x, y) &= \sum_{k_1 = \frac{-N_1}{2} + 1}^{\frac{N_1}{2}} \sum_{k_2 = \frac{-N_2}{2} + 1}^{\frac{N_2}{2}} \hat{\rho}_{k_1, k_2} e^{i(k_1 x + k_2 y)}, \\
 &\quad k_1 = \frac{-N_1}{2} + 1 \quad k_2 = \frac{-N_2}{2} + 1
 \end{aligned}$$

showing that  $\vec{k}$  space structure contains only  $N_1 \times N_2$  independent points

(see Fig. 24). The amplitudes  $\hat{\rho}_{k_1, k_2}$  can be obtained from

$$\begin{aligned}
 \rho_{i, j}^0 &= \sum_{k_1 = \frac{-N_1}{2} + 1}^{\frac{N_1}{2}} \sum_{k_2 = \frac{-N_2}{2} + 1}^{\frac{N_2}{2}} \hat{\rho}_{k_1, k_2} e^{i\left(\frac{2\pi k_1 i\delta x}{L_1} + \frac{2\pi k_2 j\delta y}{L_2}\right)} \quad (214) \\
 &\quad k_1 = \frac{-N_1}{2} + 1 \quad k_2 = \frac{-N_2}{2} + 1
 \end{aligned}$$

for  $i = 0, 1, 2, \dots, N_1 - 1$ , and  $j = 0, 1, 2, \dots, N_2 - 1$ .

In terms of sines and cosines, Eq. (213) can be written as

$$\begin{aligned}
f(x,y) = & A_{0,0} + \left( \sum_{k_1=1}^{\frac{N_1}{2}-1} \sum_{k_2=1}^{\frac{N_2}{2}-1} A_{k_1,k_2} \cos \left( \frac{2\pi k_1 x}{L_1} + \frac{2\pi k_2 y}{L_2} \right) \right. \\
& + B_{k_1,k_2} \sin \left( \frac{2\pi k_1 x}{L_1} + \frac{2\pi k_2 y}{L_2} \right) + C_{k_1,k_2} \cos \left( \frac{2\pi k_1 x}{L_1} - \frac{2\pi k_2 y}{L_2} \right) \\
& + D_{k_1,k_2} \sin \left( \frac{2\pi k_1 x}{L_1} - \frac{2\pi k_2 y}{L_2} \right) \left. + \sum_{k_1=1}^{\frac{N_1}{2}-1} \left( A_{k_1,0} \cos \left( \frac{2\pi k_1 x}{L_1} \right) \right. \right. \\
& + B_{k_1,0} \sin \left( \frac{2\pi k_1 x}{L_1} \right) \left. + \frac{A_{N_1,0}}{2} \cos \left( \frac{\pi N_1 x}{L_1} \right) + \sum_{k_2=1}^{\frac{N_2}{2}-1} \left( A_{0,k_2} \cos \left( \frac{2\pi k_2 y}{L_2} \right) \right. \right. \\
& + B_{0,k_2} \sin \left( \frac{2\pi k_2 y}{L_2} \right) \left. + A_{0,\frac{N_2}{2}} \cos \left( \frac{\pi N_2 y}{L_2} \right) + \frac{A_{N_1}}{2}, \frac{N_2}{2} \cos \left( \frac{\pi N_1 x}{L_1} + \frac{\pi N_2 y}{L_2} \right) \right),
\end{aligned}
\tag{215}$$

where

$$\hat{\delta}_{k_1,k_2} = \begin{cases} \frac{A_{k_1,k_2} - iB_{k_1,k_2}}{2} & \text{for } k_1 > 0, k_2 > 0 \\ \frac{A_{k_1,k_2} + iB_{k_1,k_2}}{2} & \text{for } k_1 < 0, k_2 < 0 \\ \frac{C_{k_1,k_2} - iD_{k_1,k_2}}{2} & \text{for } k_1 > 0, k_2 < 0 \\ \frac{C_{k_1,k_2} + iD_{k_1,k_2}}{2} & \text{for } k_1 < 0, k_2 > 0 \end{cases}$$

Again, we have in Eq. (215)  $N_1 \times N_2$  coefficients:  $A_{k_1, k_2}$  ( $k_1 = 0, 1, \dots, \frac{N_1}{2}$  and  $k_2 = 0, 1, \dots, \frac{N_2}{2}$ ),  $B_{k_1, k_2}$  ( $k_1 = 0, 1, \dots, \frac{N_1}{2} - 1$  and  $k_2 = 0, 1, \dots, \frac{N_2}{2} - 1$ ),  $C_{k_1, k_2}$ ,  $D_{k_1, k_2}$  ( $k_1 = 1, 2, \dots, \frac{N_1}{2} - 1$  and  $k_2 = 1, 2, \dots, \frac{N_2}{2} - 1$ ) that can be determined from the system of equations  $f(x_i, x_j) \equiv \rho_{i,j}^0$ .

Going back to Fig. 24 let us count the different harmonics. The harmonics are considered equal if they have the same magnitude

$$|\vec{k}| \equiv \sqrt{\left(\frac{2\pi k_1}{L_1}\right)^2 + \left(\frac{2\pi k_2}{L_2}\right)^2} \text{ and are aligned, i.e., } \frac{k_1}{L_1} : \frac{k_2}{L_2} = \text{constant.}$$

The number of the harmonics is almost half the space of Fig. 24 since  $(k_1, k_2)$  is equivalent to  $(-k_1, -k_2)$  and  $(k_1, -k_2)$  is equivalent to  $(-k_1, k_2)$ . For example: a and b in Fig. 24 are equivalent. Figure 25 shows the independent harmonics selected to match the choice in Eq. (215). The number of the harmonics is therefore,  $\frac{N_1 N_2}{2} + 1$ .

If we count the maximum number of wave lengths, we get an even smaller number, since according to Eq. (207a),  $\lambda = \frac{2\pi}{|\vec{k}|}$ . Two harmonics such as a and b in Fig. 25 will give the same value for  $|\vec{k}|$ . The maximum number of wave lengths is therefore  $(\frac{N_1}{2} + 1) \cdot (\frac{N_2}{2} + 1)$ , corresponding to the positive quadrant of Fig. 25. This is an upper limit. This is because the number of wave lengths can be less if the ratio  $\delta x / \delta y$  is a rational number. As explained above, decomposition in two directions puts a limit on the longest finite wave length  $\lambda$  in a given direction. Discretization, on the other hand, puts a limit on the shortest wave length in a given direction since it reduces  $n$  in Eq. (208). The largest value occurs for  $k_1 = \frac{N_1}{2}$ ,  $k_2 = \frac{N_2}{2}$ . If  $k_1^{(1)}$ ,  $k_2^{(2)}$  are the smallest integers for a given direction, the shortest wave length along this direction

corresponds to

$$n = \min_{\text{integer}} \left( \frac{N_1/2}{k_1^{(1)}}, \frac{N_2/2}{k_2^{(2)}} \right). \quad (216)$$

Assuming  $\rho(x, y, 0) = f(x, y)$ , i.e., assuming the density in between the grid points values  $\rho_{i,j}^0$  to be  $f(x, y)$ , Eq. (202) predicts the density at time  $t$  as

$$\begin{aligned} \rho(x, y, t) &= \sum_{k_1 = \frac{-N_1}{2} + 1}^{\frac{N_1}{2}} \sum_{k_2 = \frac{-N_2}{2} + 1}^{\frac{N_2}{2}} \hat{\rho}_{k_1, k_2} e^{i[k_1(x - u_1 t) + k_2(y - u_2 t)]} \\ &= \sum_{k_1} \sum_{k_2} \hat{\rho}_{k_1, k_2}(t) e^{i(k_1 x + k_2 y)} \end{aligned}$$

where  $\hat{\rho}_{k_1, k_2}(t) = \hat{\rho}_{k_1, k_2} e^{-i(k_1 u_1 t + k_2 u_2 t)}$ . Since we are only concerned

with  $\rho(x_i, y_j, t)$ , let  $x = x_i = i\delta x$ ,  $y = y_j = j\delta y$ . We then get

$$\rho(x_i, y_j, t) = \sum_{k_1 = \frac{-N_1}{2} + 1}^{\frac{N_1}{2}} \sum_{k_2 = \frac{-N_2}{2} + 1}^{\frac{N_2}{2}} \hat{\rho}_{k_1, k_2}(t) e^{i(k_1 i\delta x + k_2 j\delta y)}. \quad \text{If the time}$$

is also discretized, let  $t^n \equiv n\delta t$ ,  $\rho_{i,j}^n \equiv \rho(x_i, y_j, t^n)$  and  $\hat{\rho}_{k_1, k_2}^n \equiv \hat{\rho}_{k_1, k_2}(t^n)$ .

$$\text{Then } \rho_{i,j}^n = \sum_{k_1} \sum_{k_2} \hat{\rho}_{k_1, k_2}^n e^{i(k_1 i\delta x + k_2 j\delta y)} \quad (217)$$

where

$$\hat{\rho}_{k_1, k_2}^n = \hat{\rho}_{k_1, k_2} e^{-i(k_1 u_1 + k_2 u_2)n\delta t} \quad (218)$$

We define  $A(k_1, k_2)$  as

$$A(k_1, k_2) = \frac{\rho_{k_1, k_2}^{n+1}}{\delta_{k_1, k_2}^n}.$$

Equation (218) expresses the analytic solution as

$$A(k_1, k_2) = e^{-i(k_1 u_1 \delta t + k_2 u_2 \delta t)}. \quad (219)$$

If we denote  $\frac{u_1 \delta t}{\delta x}$  by  $\epsilon_x$ ,  $\frac{u_2 \delta t}{\delta y}$  by  $\epsilon_y$ ,  $k_1 \delta x$  by  $\beta_x$ , and  $k_2 \delta y$  by  $\beta_y$ , Eq. (219) reduces to

$$A(k_1, k_2) = e^{-i(\epsilon_x \beta_x + \epsilon_y \beta_y)} \quad (220)$$

Now let us analyze a fully two-dimensional scheme, a direct extension of the one-dimensional scheme

$$\begin{aligned} \rho_j^T &= \rho_j^n - \frac{\epsilon}{2}(\rho_{j+1}^n - \rho_{j-1}^n) \\ \rho_j^{TD} &= \rho_j^T + v(\rho_{j+1}^n - 2\rho_j^n + \rho_{j-1}^n) \\ \rho_j^{n+1} &= \rho_j^{TD} - u(\rho_{j+1}^T - 2\rho_j^T + \rho_{j-1}^T), \end{aligned} \quad (221)$$

namely,

$$\rho_{i,j}^{Tx} = \rho_{i,j}^n - \frac{\epsilon_x}{2}(\rho_{i+1,j}^n - \rho_{i-1,j}^n); \quad (222a)$$

$$\rho_{i,j}^{Ty} = \rho_{i,j}^n - \frac{\epsilon_y}{2}(\rho_{i,j+1}^n - \rho_{i,j-1}^n); \quad (222b)$$

$$\rho_{i,j}^T = \rho_{i,j}^n - \frac{\epsilon_x}{2}(\rho_{i+1,j}^n - \rho_{i-1,j}^n) - \frac{\epsilon_y}{2}(\rho_{i,j+1}^n - \rho_{i,j-1}^n); \quad (222c)$$

$$\begin{aligned} \rho_{i,j}^{TD} &= \rho_{i,j}^T + v_x(\rho_{i+1,j}^n - 2\rho_{i,j}^n + \rho_{i-1,j}^n) + v_y(\rho_{i,j+1}^n - 2\rho_{i,j}^n \\ &\quad + \rho_{i,j-1}^n); \end{aligned} \quad (222d)$$

$$\rho_{i,j}^{n+1} = \rho_{i,j}^{TD} - \mu_x (\rho_{i+1,j}^{Tx} - 2\rho_{i,j}^{Tx} + \rho_{i-1,j}^{Tx}) - \mu_y (\rho_{i,j+1}^{Ty} - 2\rho_{i,j}^{Ty} + \rho_{i,j-1}^{Ty}). \quad (222e)$$

Again as in one-dimension, after Fourier-analyzing the initial density profile, i.e., after we have gotten the  $\{\hat{\rho}_{k_1, k_2}\}$ , the problem is reduced to propagation of the complex harmonics  $e^{i(k_1 x + k_2 y)}$ . Since for the linear problem Eq. (201), each harmonic propagates independently, we can get  $A(k_1, k_2)$  by assuming only one harmonic:

$$\rho_{i,j}^n = \rho^n e^{i(k_1 i \delta x + k_2 j \delta y)} = \rho^n e^{i(i \beta_x + j \beta_y)}, \quad (223)$$

then using

$$A(k_1, k_2) = \frac{\rho_{i,j}^{n+1}}{\rho_{i,j}^n}. \quad (224)$$

Substituting Eq. (223) into (222a) we get

$$\begin{aligned} \rho_{i,j}^{Tx} &= \rho^n e^{i(k_1 i \delta x + k_2 j \delta y)} - \frac{\epsilon_x}{2} \{ \rho^n e^{i[k_1 (i+1) \delta x + k_2 j \delta y]} \\ &\quad - \rho^n e^{i[k_1 (i-1) \delta x + k_2 j \delta y]} \} \end{aligned} \quad (225)$$

hence

$$\frac{\rho_{i,j}^{Tx}}{\rho_{i,j}^n} = 1 - \frac{\epsilon_x}{2} (e^{i \beta_x} - e^{-i \beta_x}) = 1 - i \epsilon_x \sin \beta_x \quad (226a)$$

Similarly Eq. (222b) gives

$$\frac{\rho_{i,j}^{Ty}}{\rho_{i,j}^n} = 1 - i \epsilon_y \sin \beta_y. \quad (226b)$$

Denoting  $i \sin \beta_x$  by  $t_x$  and  $i \sin \beta_y$  by  $t_y$ , Eq. (222c) gives

$$\frac{\rho_{i,j}^T}{\rho_{i,j}^n} = 1 - \epsilon_x t_x - \epsilon_y t_y \quad (226c)$$

Substituting Eq. (223) into (222d)

$$\begin{aligned} \frac{\rho_{i,j}^{TD}}{\rho_{i,j}^n} &= \frac{\rho_{i,j}^T}{\rho_{i,j}^n} + v_x (e^{i\beta_x} - 2 + e^{-i\beta_x}) + v_y (e^{i\beta_y} - 2 + e^{-i\beta_y}) \\ &= \frac{\rho_{i,j}^T}{\rho_{i,j}^n} + v_x d_x + v_y d_y, \end{aligned} \quad (226d)$$

where  $d_x \equiv 2(\cos \beta_x - 1)$  and  $d_y \equiv 2(\cos \beta_y - 1)$ . Finally, Eq. (222e) yields with Eqs. (226c) and (226d)

$$\begin{aligned} A(\beta_x, \beta_y) &= \frac{\rho_{i,j}^{n+1}}{\rho_{i,j}^n} = (1 - \epsilon_x t_x - \epsilon_y t_y) + v_x d_x + v_y d_y - \mu_x d_x (1 - \epsilon_x t_x) \\ &\quad - \mu_y d_y (1 - \epsilon_y t_y) \end{aligned} \quad (226e)$$

From which

$$\rho_{i,j}^{n+1} = A(\beta_x, \beta_y) \rho_{i,j}^0 e^{i(i\beta_x + j\beta_y)}$$

We notice that the coefficient of  $e^{i(i\beta_x + j\beta_y)}$  is independent of  $i$  and  $j$ , i.e., independent of  $x, y$ . Consequently,  $\rho_{i,j}^{n+1}$  have the same wave front inclination and shape as  $\rho_{i,j}^n$ ; i.e., along the lines of  $k_1 x + k_2 y = \text{constant}$ ,  $\rho_{i,j}^{n+1} = \text{constant}$ . Finally, this is a nine-point explicit scheme, as illustrated in Fig. 26, which shows the points involved in determining  $\rho_{i,j}^{n+1}$ .

## XII. AMPLITUDE AND PHASE ANALYSIS

We write  $A$  as  $A = |A|e^{i\theta}$ , where  $|A|$  is the amplitude and  $\theta$  is the phase angle. To classify the order of the scheme we need to expand  $|A|$  and  $\theta$  in a power series in  $\beta_x$  and  $\beta_y$ .

### PHASE ERRORS

In the two-dimensional case we have  $A = A(t_x, t_y, d_x, d_y)$  where  $t_x, d_x$  are functions of  $\beta_x$ , while  $t_y, d_y$  are functions of  $\beta_y$ . Since  $\log A = \log |A| + i(\theta)$ ,

$$\theta = \text{Im} (\log A). \quad (229)$$

Expanding  $\theta$  in a power series of  $\beta_x, \beta_y$  near  $\beta_x, \beta_y = 0$ , we get

$$\theta = \theta_0 + (\theta_0^x \beta_x + \theta_0^y \beta_y) + (\theta_0^{xx} \frac{\beta_x^2}{2} + \theta_0^{xy} \beta_x \beta_y + \theta_0^{yy} \frac{\beta_y^2}{2}) \quad (230)$$

$$+ (\theta_0^{xxx} \frac{\beta_x^3}{6} + \theta_0^{xxy} \frac{\beta_x^2 \beta_y}{2} + \theta_0^{xyy} \frac{\beta_x \beta_y^2}{2} + \theta_0^{yyy} \frac{\beta_y^3}{6}) + \dots, \quad (230)$$

where  $\theta_0^x \equiv (\partial\theta/\partial\beta_x)$  at  $\beta_x = 0$ , while  $\theta_0^y \equiv (\partial\theta/\partial\beta_y)$  at  $\beta_y = 0$ , etc.

We therefore need the derivatives of  $\log A$ . Noticing that  $A(\beta_x, \beta_y = 0) = 1$  we get

$$(\log A)_0^x = A_0^x \quad (231a)$$

$$(\log A)_0^y = A_0^y; \quad (231b)$$

$$(\log A)_0^{xx} = A_0^{xx} - (A_0^x)^2; \quad (232a)$$

$$(\log A)_0^{xy} = A_0^{xy} - A_0^x A_0^y; \quad (232b)$$



$$(\log A)_o^{YY} = A_o^{YY} - (A_o^Y)^2 \quad (232c)$$

$$(\log A)_o^{xxx} = A_o^{xxx} - 3A_o^{xx}A_o^x + 2(A_o^x)^3; \quad (233a)$$

$$(\log A)_o^{xxy} = A_o^{xxy} - 2A_o^{xy}A_o^x - A_o^{xx}A_o^y + 2(A_o^x)^2A_o^y; \quad (233b)$$

$$(\log A)_o^{xyy} = A_o^{xyy} - 2A_o^{xy}A_o^y - A_o^{xx}A_o^{yy} + 2A_o^x(A_o^y)^2; \quad (233c)$$

$$(\log A)_o^{yyy} = A_o^{yyy} - 3A_o^{yy}A_o^y + 2(A_o^y)^3; \quad (233d)$$

and so on.

Denoting  $\frac{\partial(\ )}{\partial t_x} |_{\beta_x, \beta_y} = 0$  by  $(\ )_o^x$ ,  $\frac{\partial(\ )}{\partial d_x} |_{\beta_x, \beta_y} = 0$  by  $(\ )_o^d$ ,

so on, confining our scope to schemes of second degree in the operators

$t_x, t_y, d_x$ , or  $d_y$ , and using the chain rule of differentiation we get

$$A_o^x = A_o^x t_{xo}' + A_o^x d_{xo}'; \quad (235a)$$

$$A_o^y = A_o^y t_{yo}' + A_o^y d_{yo}'; \quad (235b)$$

$$A_o^{xx} = t_{xo}'' A_o^x + d_{xo}'' A_o^x + t_{xo}^{'2} A_o^{xx} + 2t_{xo}' d_{xo}' A_o^{xx} + d_{xo}^{'2} A_o^{xx}; \quad (236a)$$

$$A_o^{xy} = t_{xo}' t_{yo}' A_o^{xy} + t_{xo}' d_{yo}' A_o^{xy} + d_{xo}' t_{yo}' A_o^{xy} + d_{xo}' d_{yo}' A_o^{xy}; \quad (236b)$$

$$A_o^{yy} = t_{yo}'' A_o^y + d_{yo}'' A_o^y + t_{yo}^{'2} A_o^{yy} + 2t_{yo}' d_{yo}' A_o^{yy} + d_{yo}^{'2} A_o^{yy}; \quad (236c)$$

$$A_o^{xxx} = t_{xo}^{'''} A_o^x + d_{xo}^{'''} A_o^x + 3t_{xo}'' t_{xo}' A_o^{xx} + 3(t_{xo}' d_{xo}'' + t_{xo}'' d_{xo}') A_o^{xx} + 3d_{xo}' d_{xo}'' A_o^{xx}; \quad (237a)$$

$$A_o^{xxy} = t_{xo}'' t_{yo}' A_o^{xy} + t_{xo}' d_{yo}'' A_o^{xy} + d_{xo}'' t_{yo}' A_o^{xy} + d_{xo}' d_{yo}'' A_o^{xy}; \quad (237b)$$

$$A_{\text{O}}^{\text{xyy}} = t_{\text{xO}}' t_{\text{yO}}'' A_{\text{O}}^{\text{xy}} + t_{\text{xO}}' d_{\text{yO}}'' A_{\text{O}}^{\text{xy}} + d_{\text{xO}}' t_{\text{yO}}'' A_{\text{O}}^{\text{xy}} + d_{\text{xO}}' d_{\text{yO}}'' A_{\text{O}}^{\text{xy}}; \quad (237c)$$

$$A_{\text{O}}^{\text{yyy}} = t_{\text{yO}}''' A_{\text{O}}^{\text{y}} + d_{\text{yO}}''' A_{\text{O}}^{\text{y}} + 3t_{\text{yO}}' t_{\text{yO}}'' A_{\text{O}}^{\text{yy}} \\ + 3(t_{\text{yO}}' d_{\text{yO}}'' + t_{\text{yO}}'' d_{\text{yO}}') A_{\text{O}}^{\text{yy}} + 3d_{\text{yO}}' d_{\text{yO}}'' A_{\text{O}}^{\text{yy}}. \quad (237d)$$

Finally,

$$A_{\text{O}}^{\text{xxxx}} = t_{\text{xO}}^{\text{iv}} A_{\text{O}}^{\text{x}} + d_{\text{xO}}^{\text{iv}} A_{\text{O}}^{\text{x}} + (4t_{\text{xO}}' t_{\text{xO}}''' + 3t_{\text{xO}}''^2) A_{\text{O}}^{\text{xx}} + (4t_{\text{xO}}' d_{\text{xO}}' \\ + 6t_{\text{xO}}'' d_{\text{xO}}'' + 4t_{\text{xO}}' d_{\text{xO}}''') A_{\text{O}}^{\text{xx}} + (4d_{\text{xO}}' d_{\text{xO}}''' + 3d_{\text{xO}}''^2) A_{\text{O}}^{\text{xx}}; \quad (239a)$$

$$A_{\text{O}}^{\text{xxxy}} = t_{\text{xO}}''' (t_{\text{yO}}' A_{\text{O}}^{\text{xy}} + d_{\text{yO}}' A_{\text{O}}^{\text{xy}}) + d_{\text{xO}}''' (t_{\text{yO}}' A_{\text{O}}^{\text{xy}} + d_{\text{yO}}' A_{\text{O}}^{\text{xy}}); \quad (239b)$$

$$A_{\text{O}}^{\text{xxyy}} = t_{\text{xO}}'' t_{\text{yO}}'' A_{\text{O}}^{\text{xy}} + d_{\text{xO}}'' d_{\text{yO}}'' A_{\text{O}}^{\text{xy}} + t_{\text{xO}}'' d_{\text{yO}}'' A_{\text{O}}^{\text{xy}} + d_{\text{xO}}'' t_{\text{yO}}'' A_{\text{O}}^{\text{xy}}; \quad (239c)$$

$$A_{\text{O}}^{\text{xyyy}} = t_{\text{yO}}''' (t_{\text{xO}}' A_{\text{O}}^{\text{xy}} + d_{\text{xO}}' A_{\text{O}}^{\text{xy}}) + d_{\text{yO}}''' (t_{\text{xO}}' A_{\text{O}}^{\text{xy}} + d_{\text{xO}}' A_{\text{O}}^{\text{xy}}); \quad (239d)$$

$$A_{\text{O}}^{\text{yyyy}} = t_{\text{yO}}^{\text{iv}} A_{\text{O}}^{\text{y}} + d_{\text{yO}}^{\text{iv}} A_{\text{O}}^{\text{y}} + (4t_{\text{yO}}' t_{\text{yO}}''' + 3t_{\text{yO}}''^2) A_{\text{O}}^{\text{yy}} - (4t_{\text{yO}}' d_{\text{yO}}' \\ + 6t_{\text{yO}}'' d_{\text{yO}}'' + 4t_{\text{yO}}' d_{\text{yO}}''') A_{\text{O}}^{\text{yy}} + (4d_{\text{yO}}' d_{\text{yO}}''' + 3d_{\text{yO}}''^2) A_{\text{O}}^{\text{yy}}; \quad (239e)$$

Going back to the definitions of  $t_{\text{x}}, t_{\text{y}}, d_{\text{x}},$  and  $d_{\text{y}},$

$$t_{\text{xO}} = t_{\text{yO}} = 0;$$

$$t_{\text{xO}}' = t_{\text{yO}}' = i;$$

$$t_{\text{xO}}'' = t_{\text{yO}}'' = 0;$$

$$t_{\text{xO}}''' = t_{\text{yO}}''' = -i;$$

$$t_{\text{xO}}^{\text{iv}} = t_{\text{yO}}^{\text{iv}} = 0;$$

(240a)

$$d_{xo} = d_{yo} = 0;$$

$$d'_{xo} = d'_{yo} = 0;$$

$$d''_{xo} = d''_{yo} = -2;$$

(240b)

$$d'''_{xo} = d'''_{yo} = 0;$$

$$d^{iv}_{xo} = d^{iv}_{yo} = 2.$$

Substituting into Eqs. (235)-(239) and assuming  $A^{txx} = A^{tyy} = 0$ , we get

$$A_o = 1; \quad (241)$$

$$A_o^x = iA_o^t, \quad A_o^y = iA_o^t; \quad (242)$$

$$A_o^{xx} = -2A_o^d, \quad A_o^{xy} = -A_o^{txy}, \quad A_o^{yy} = -2A_o^d; \quad (243)$$

$$A_o^{xxx} = -i(A_o^t + 6A_o^{dx}); \quad (244a)$$

$$A_o^{xxy} = -2iA_o^{tdx}; \quad (244b)$$

$$A_o^{xyy} = -2iA_o^{tdy}; \quad (244c)$$

$$A_o^{yyy} = -i(A_o^t + 6A_o^{tdy}); \quad (244d)$$

and

$$A_o^{xxxx} = 2(A_o^d + 6A_o^{dx}); \quad (245a)$$

$$A_o^{xxyy} = A_o^{txy}; \quad (245b)$$

$$A_o^{xyyy} = 4A_o^{tdy}; \quad (245c)$$

$$A_o^{yyyy} = A_o^{tdy}; \quad (245d)$$

$$A_{\circ}^{YYYY} = 2(A_{\circ}^Y + 6A_{\circ}^{dY}). \quad (245e)$$

It is worth noticing that Eqs. (241)-(244) are valid for schemes of higher degree in the operators  $t_x, t_y, d_x$ , and  $d_y$ , as long as  $A_{\circ}^{t_x t_x} = A_{\circ}^{t_y t_y} = 0$ , i.e., as long as composite transport is excluded. With the above equations, Eqs. (231)-(233) yield

$$(\log A)_{\circ}^x = iA_{\circ}^{t_x}, \quad (\log A)_{\circ}^y = iA_{\circ}^{t_y}; \quad (246)$$

$$(\log A)_{\circ}^{xx} = -2A_{\circ}^{d_x} + (A_{\circ}^{t_x})^2; \quad (247a)$$

$$(\log A)_{\circ}^{xy} = -A_{\circ}^{t_x t_y} + A_{\circ}^{t_x} A_{\circ}^{t_y}; \quad (247b)$$

$$(\log A)_{\circ}^{yy} = -2A_{\circ}^{d_y} + (A_{\circ}^{t_y})^2; \quad (247c)$$

$$(\log A)_{\circ}^{xxx} = -iA_{\circ}^{t_x}(1 - 6A_{\circ}^{d_x}) - i[6A_{\circ}^{t_x d_x} + 2(A_{\circ}^{t_x})^3]; \quad (248a)$$

$$(\log A)_{\circ}^{xxy} = -2i(A_{\circ}^{d_x t_y} - A_{\circ}^{d_x} A_{\circ}^{t_y} + 2iA_{\circ}^{t_x}(A_{\circ}^{t_x t_y} - A_{\circ}^{t_x} A_{\circ}^{t_y})); \quad (248b)$$

$$(\log A)_{\circ}^{xyy} = -2i(A_{\circ}^{d_y t_x} - A_{\circ}^{d_y} A_{\circ}^{t_x}) + 2iA_{\circ}^{t_y}(A_{\circ}^{t_x t_y} - A_{\circ}^{t_x} A_{\circ}^{t_y}); \quad (248c)$$

$$(\log A)_{\circ}^{yyy} = -iA_{\circ}^{t_y}(1 - 6A_{\circ}^{d_y}) - i[6A_{\circ}^{t_y d_y} + 2(A_{\circ}^{t_y})^3]. \quad (248d)$$

Only the odd derivatives are imaginary. Therefore, Eq. (229) implies

$$\begin{aligned} \partial = & \left[ \frac{(\log A)_{\circ}^x}{i} \beta_x + \frac{(\log A)_{\circ}^y}{i} \beta_y \right] + \left[ \frac{(\log A)_{\circ}^{xxx}}{i} \frac{\beta_x^3}{6} \right. \\ & \left. + \frac{(\log A)_{\circ}^{xxy}}{i} \frac{\beta_x^2 \beta_y}{2} + \frac{(\log A)_{\circ}^{xyy}}{i} \frac{\beta_x \beta_y^2}{2} + \frac{(\log A)_{\circ}^{yyy}}{i} \frac{\beta_y^3}{6} \right] + \dots \quad (249) \end{aligned}$$

Example:

Let us analyze the phase error associated with Eq. (226e),

$$A = (1 - \epsilon_x t_x - \epsilon_y t_y) + v_x d_x + v_y d_y - \mu_x d_x (1 - \epsilon_x t_x) - \mu_y d_y (1 - \epsilon_y t_y).$$

By direct differentiation we get

$$A_o^t x = \epsilon_x, \quad A_o^t y = -\epsilon_y; \quad (250)$$

$$A_o^d x = v_x - \mu_x, \quad A_o^d y = v_y - \mu_y;$$

$$A_o^{t t} x = 0, \quad A_o^{t d} x = \epsilon_x \mu_x, \quad A_o^{d d} x = 0;$$

$$A_o^{t t} y = 0, \quad A_o^{t d} y = \epsilon_y \mu_y, \quad A_o^{d d} y = 0;$$

$$A_o^{t t} y = 0, \quad A_o^{t d} y = 0, \quad A_o^{t d} x = 0, \quad A_o^{d d} y = 0;$$

whence

$$\frac{(\log A)_o^x}{i} = -\epsilon_x, \quad \frac{(\log A)_o^y}{i} = -\epsilon_y; \quad (251)$$

$$\frac{(\log A)_o^{xxx}}{i} = 6\epsilon_x \left( \frac{1}{6} - v_x + \frac{\epsilon_x^2}{3} \right) \quad (252a)$$

$$\frac{(\log A)_o^{xxy}}{i} = -2\epsilon_y (v_x - \mu_x - \epsilon_x^2); \quad (252b)$$

$$\frac{(\log A)_o^{xyy}}{i} = -2\epsilon_x (v_y - \mu_y - \epsilon_y^2); \quad (252c)$$

$$\frac{(\log A)_o^{yyy}}{i} = 6\epsilon_y \left( \frac{1}{6} - v_y + \frac{\epsilon_y^2}{3} \right). \quad (252d)$$

Substituting in Eq. (249), we get

$$\begin{aligned} \theta = & -\epsilon_x \beta_x \left[ 1 + \left( v_x - \frac{1}{6} - \frac{\epsilon_x^2}{3} \right) \beta_x^2 + (v_y - \mu_y - \epsilon_y^2) \beta_y^2 + \dots \right] \\ & - \epsilon_y \beta_y \left[ 1 + \left( v_y - \frac{1}{6} - \frac{\epsilon_y^2}{3} \right) \beta_y^2 + (v_x - \mu_x - \epsilon_x^2) \beta_x^2 + \dots \right]. \end{aligned}$$

Noting that  $\epsilon_x \beta_x = \left(\frac{u_1 \delta t}{\delta x}\right) (k_1 \delta x) = u_1 k_1 \delta t$  and  $\epsilon_y \beta_y = u_2 k_2 \delta t$ , we can rewrite the above equation as

$$\vartheta = -\vec{k} \cdot \vec{V} \delta t, \quad (253)$$

where  $\vec{k} = (k_1, k_2)$ ,  $\vec{V} = (v_1, v_2)$ . If  $\vec{U} = (u_1, u_2)$ ,

$$v_1 = u_1 \left[ 1 + \left( v_x - \frac{1}{6} - \frac{\epsilon_x^2}{3} \right) \beta_x^2 + \left( v_y - u_y - \epsilon_y^2 \right) \beta_y^2 + \dots \right];$$

and

$$v_2 = u_2 \left[ 1 + \left( v_y - \frac{1}{6} - \frac{\epsilon_y^2}{3} \right) \beta_y^2 + \left( v_x - u_x - \epsilon_x^2 \right) \beta_x^2 + \dots \right]. \quad (254b)$$

Comparing Eq. (253) to the analytical solution, we find

$$\vartheta_{\text{analytic}} = -\vec{k} \cdot \vec{U} \delta t \quad (255)$$

as is obvious from Eqs. (211).

Following Eq. (19b), we define a relative phase error matrix,  $R$ , such that

$$\vec{V} = \vec{U} + R\vec{U}, \quad (256)$$

where  $R$ , given by Eqs. (254), in this scheme is

$$R = \begin{pmatrix} \left( v_x - \frac{1}{6} - \frac{\epsilon_x^2}{3} \right) \beta_x^2 + \left( v_y - u_y - \epsilon_y^2 \right) \beta_y^2 & \dots & 0 \\ 0 & \left( v_y - \frac{1}{6} - \frac{\epsilon_y^2}{3} \right) \beta_y^2 + \left( v_x - u_x - \epsilon_x^2 \right) \beta_x^2 & \dots \end{pmatrix}, \quad (257)$$

Thus we can reduce the phase error to fourth order by selecting

$$v_{\frac{x}{y}} = \frac{1}{6} + \epsilon_{\frac{x}{y}}^2 / 3; \quad (258a)$$

$$v_{\frac{x}{y}} - u_{\frac{x}{y}} = \epsilon_{\frac{x}{y}}^2. \quad (258b)$$

Solving Eqs. (258a, b), we get

$$\mu_{\frac{x}{y}} = \frac{1}{6} - \frac{2}{3} \epsilon_{\frac{x}{y}}^2. \quad (258c)$$

### AMPLITUDE ANALYSIS

Following the analysis of the one-dimensional case, since  $|A|^2 = A\bar{A}$  we have

$$\begin{aligned} (|A|^2)_0 &= 1; \\ (|A|^2)_0^x &= A_0^x \bar{A}_0^x + A_0 \bar{A}_0^x, \\ (|A|^2)_0^y &= A_0^y \bar{A}_0^y + A_0 \bar{A}_0^y, \end{aligned} \quad (259)$$

and so on. Noticing from Eqs. (241)-(245) that odd derivatives are purely imaginary while even ones are real, we get after substituting in Eqs. (259)

$$(|A|^2)_0 = 1; \quad (260)$$

$$(|A|^2)_0^{xx} = 2[A_0^{xx} + (\frac{A_0^x}{i})^2]; \quad (261a)$$

$$(|A|^2)_0^{xy} = 2[A_0^{xy} + \frac{A_0^x}{i} \frac{A_0^y}{i}]; \quad (261b)$$

$$(|A|^2)_0^{yy} = 2[A_0^{yy} + (\frac{A_0^y}{i})^2]; \quad (261c)$$

$$(|A|^2)_0^{xxxx} = 2[A_0^{xxxx} + 4(\frac{A_0^x}{i})(\frac{A_0^{xy}}{i}) + 3(A_0^{xx})^2]; \quad (262a)$$

$$(|A|^2)_0^{xxyy} = 2[A_0^{xxyy} + (\frac{A_0^{xxx}}{i})(\frac{A_0^y}{i}) + 3(\frac{A_0^{xy}}{i})(\frac{A_0^x}{i}) + (3A_0^{xx}A_0^{xy})]; \quad (262b)$$

$$\begin{aligned} (|A|^2)_0^{xxyy} &= 2[A_0^{xxyy} + (\frac{A_0^{xxy}}{i})(\frac{A_0^y}{i}) + A_0^{xx}A_0^{yy} \\ &\quad + 2(\frac{A_0^{xyy}}{i})(\frac{A_0^x}{i}) + 2(A_0^{xy})^2]; \end{aligned} \quad (262c)$$

$$(|A|^2)_{\circ}^{xyyy} = 2[A_{\circ}^{xyyy} + (\frac{A_{\circ}^x}{i})(\frac{A_{\circ}^{yyy}}{i}) + 3(\frac{A_{\circ}^{xyy}}{i})(\frac{A_{\circ}^y}{i}) + 3A_{\circ}^{xy}A_{\circ}^{yy}]; \quad (262d)$$

$$(|A|^2)_{\circ}^{yyyy} = 2[A_{\circ}^{yyyy} + 4(\frac{A_{\circ}^y}{i})(\frac{A_{\circ}^{yyy}}{i}) + 3(A_{\circ}^{yy})^2], \quad (262e)$$

while the odd derivative vanishes. Consequently, the expansion of  $|A|^2$  takes the form

$$\begin{aligned} |A|^2 = & (|A|^2)_{\circ} + [(|A|^2)_{\circ}^{xx} \frac{\beta_x^2}{2} + (|A|^2)_{\circ}^{xy} \beta_x \beta_y + (|A|^2)_{\circ}^{yy} \frac{\beta_y^2}{2}] \\ & + [(|A|^2)_{\circ}^{xxxx} \frac{\beta_x^4}{24} + (|A|^2)_{\circ}^{xxxy} \frac{\beta_x^3 \beta_y}{6} + (|A|^2)_{\circ}^{xxyy} \frac{\beta_x^2 \beta_y^2}{4} \\ & + (|A|^2)_{\circ}^{xyyy} \frac{\beta_x \beta_y^3}{6} + (|A|^2)_{\circ}^{yyyy} \frac{\beta_y^4}{24}] + \dots \end{aligned} \quad (263)$$

Example:

Using Eqs. (250), Eqs. (241)-(243) yield

$$A_{\circ} = 1;$$

$$\frac{A_{\circ}^x}{i} = -\epsilon_x, \quad \frac{A_{\circ}^y}{i} = -\epsilon_y;$$

$$A_{\circ}^{xx} = -2(v_x - \mu_x) = -2\epsilon_x^2;$$

$$A_{\circ}^{xy} = 0;$$

$$A_{\circ}^{yy} = -2(v_y - \mu_y) = -2\epsilon_y^2,$$

which when substituted into Eqs. (260), (261) give

$$(|A|^2)_{\circ} = 1;$$

$$(|A|^2)_{\circ}^{xx} = -2\epsilon_x^2;$$



$$(|A|^2)_0^{xy} = 2\varepsilon_x \varepsilon_y;$$

$$(|A|^2)_0^{yy} = -2\varepsilon_y^2.$$

Equation (263) then expresses the amplitude expansion as

$$\begin{aligned} |A|^2 &= 1 - (\varepsilon_x^2 \beta_x^2 - 2\varepsilon_x \varepsilon_y \beta_x \beta_y + \varepsilon_y^2 \beta_y^2) + \dots \\ |A|^2 &= 1 = -|\varepsilon_x \beta_x - \varepsilon_y \beta_y|^2 + \dots, \end{aligned} \quad (264)$$

showing that the diffusion of the scheme is second-order.

### POSITIVITY

From Eqs. (223) and using Eq. (258a),

$$\begin{aligned} \rho_{i,j}^{TD} &= \rho_{i,j}^n [1 - 2(\frac{1}{6} + \frac{\varepsilon_x^2}{3}) - 2(\frac{1}{6} + \frac{\varepsilon_y^2}{3})] \\ &+ \rho_{i+1,j}^n [\frac{1}{6} + \frac{\varepsilon_x^2}{3} - \frac{\varepsilon_x}{2}] + \rho_{i-1,j}^n [\frac{1}{6} + \frac{\varepsilon_x^2}{3} + \frac{\varepsilon_x}{2}] \\ &+ \rho_{i,j+1}^n [\frac{1}{6} + \frac{\varepsilon_y^2}{3} - \frac{\varepsilon_y}{2}] + \rho_{i,j-1}^n [\frac{1}{6} + \frac{\varepsilon_y^2}{3} + \frac{\varepsilon_y}{2}] \end{aligned}$$

Each of the square brackets is  $\geq 0$  for  $|\varepsilon_x|, |\varepsilon_y| \leq \frac{1}{2}$ .

Consequently,  $\rho_{i,j}^{TD} \geq 0$  if all  $\rho_{i,j}^n \geq 0$ . Now we get

$$\rho_{i,j}^{n+1} = \rho_{i,j}^{TD} - \mu_x (\rho_{i+1,j}^{T_x} - 2\rho_{i,j}^{T_x} + \rho_{i-1,j}^{T_x})^* - \mu_y (\rho_{i,j+1}^{T_y} - 2\rho_{i,j}^{T_y} + \rho_{i,j-1}^{T_y})^*$$

The asterisks denote the fact that the antidiffusion fluxes are trimmed

enough such that  $\rho_{i,j}^{n+1}$  is limited by the sign of  $\rho_{i,j}^{TD}$ . Then  $\rho_{i,j}^{n+1} \geq 0$ .

## STABILITY

Equation (264) proves the stability of the scheme near  $\beta_x = \beta_y = 0$ . For the scheme to be completely stable, however, we must have  $|A| \leq 1$  for  $0 \leq \beta_x, \beta_y \leq \pi$ . Let us check  $A$ , at the largest values admitted for  $\varepsilon_x, \varepsilon_y$ , namely  $1/2$ .

From Eq. (226e)

$$A_R = 1 - 2(v_x - u_x)(1 - \cos \beta_x) - 2(v_y - u_y)(1 - \cos \beta_y); \quad (266a)$$

$$\begin{aligned} A_I = & -\varepsilon_x \sin \beta_x [1 + 2u_x(1 - \cos \beta_x)] \\ & - \varepsilon_y \sin \beta_y [1 + 2u_y(1 - \cos \beta_y)] \end{aligned} \quad (266b)$$

Substituting for  $v_x - u_x$  from Eq. (258b), and  $u_x$  from Eq. (258c), we get

$$A_R = 1 - 2\varepsilon_x^2(1 - \cos \beta_x) - 2\varepsilon_y^2(1 - \cos \beta_y); \quad (267a)$$

$$\begin{aligned} A_I = & -\varepsilon_x \sin \beta_x [1 + \frac{1}{4}(1 - 4\varepsilon_x^2)(1 - \cos \beta_x)] \\ & - \varepsilon_y \sin \beta_y [1 + \frac{1}{4}(1 - 4\varepsilon_y^2)(1 - \cos \beta_y)]. \end{aligned} \quad (267b)$$

At  $\varepsilon_x, \varepsilon_y = 1/2$ ,  $u_x = u_y = 0$ ; Eqs. (267) reduce to

$$A_R = 1 - \frac{1}{2}(1 - \cos \beta_x) - \frac{1}{2}(1 - \cos \beta_y);$$

$$A_I = -\frac{1}{2}(\sin \beta_x + \sin \beta_y).$$

Noticing that  $1 - \cos \beta = 2 \sin^2(\beta/2)$  and  $\sin \beta = 2 \sin(\beta/2) \cos(\beta/2)$ , we get

$$A_R = 1 - \sin^2(\beta_x/2) \sin^2(\beta_y/2);$$

$$A_I = - [\sin(\beta_x/2) \cos(\beta_x/2) + \sin(\beta_y/2) \cos(\beta_y/2)],$$

yielding

$$\begin{aligned} |A|^2 &= A_R^2 + A_I^2 = 1 + \sin^4 \frac{\beta_x}{2} + \sin^4 \frac{\beta_y}{2} + 2 \sin^2 \frac{\beta_x}{2} \sin^2 \frac{\beta_y}{2} \\ &\quad - 2(\sin^2 \frac{\beta_x}{2} + \sin^2 \frac{\beta_y}{2}) + \sin^2 \frac{\beta_x}{2} \cos^2 \frac{\beta_x}{2} + \sin^2 \frac{\beta_y}{2} \cos^2 \frac{\beta_y}{2} \\ &\quad + 2 \sin \frac{\beta_x}{2} \sin \frac{\beta_y}{2} \cos \frac{\beta_x}{2} \cos \frac{\beta_y}{2}. \end{aligned}$$

Collecting the terms containing  $\sin^2 \frac{\beta_x}{2}$ , we have

$$\begin{aligned} &- \sin^2 \frac{\beta_x}{2} [(1 - \sin^2 \frac{\beta_y}{2}) + (1 - \cos^2 \frac{\beta_x}{2})] = - \sin^2 \frac{\beta_x}{2} [\cos^2 \frac{\beta_y}{2} \\ &+ \sin^2 \frac{\beta_x}{2}] = - \sin^2 \frac{\beta_x}{2} \cos^2 \frac{\beta_y}{2} - \sin^4 \frac{\beta_x}{2}. \end{aligned}$$

Similarly  $\sin^2 \frac{\beta_y}{2}$  terms yield  $- \sin^2 \frac{\beta_y}{2} \cos^2 \frac{\beta_x}{2} - \sin^4 \frac{\beta_y}{2}$ , resulting in

$$\begin{aligned} |A|^2 &= 1 - (\sin^2 \frac{\beta_x}{2} \cos^2 \frac{\beta_y}{2} - 2 \sin \frac{\beta_x}{2} \sin \frac{\beta_y}{2} \cos \frac{\beta_x}{2} \cos \frac{\beta_y}{2} \\ &\quad + \sin^2 \frac{\beta_y}{2} \cos^2 \frac{\beta_x}{2}) = 1 - (\sin \frac{\beta_x}{2} \cos \frac{\beta_y}{2} - \sin \frac{\beta_y}{2} \cos \frac{\beta_x}{2})^2 \\ &= 1 - \sin^2 (\frac{\beta_x}{2} - \frac{\beta_y}{2}) = \cos^2 (\frac{\beta_x}{2} - \frac{\beta_y}{2}). \end{aligned}$$

Consequently,

$$|A|_{\epsilon_x = \epsilon_y = \frac{1}{2}} = \cos (\frac{\beta_x}{2} - \frac{\beta_y}{2}) \leq 1, \quad (268)$$

showing the scheme to be stable at  $\epsilon_x, \epsilon_y = \frac{1}{2}$ . The value  $|A|$  for smaller values of  $\epsilon_x, \epsilon_y$  was evaluated numerically and found always to satisfy  $\leq 1$ . Hence the scheme is completely stable.

It is worth noticing the diagonal symmetry of Eqs. (264), (268). In fact, on the  $\beta_x, \beta_y$  plane,  $|A|$  looks like a wave with front parallel to the  $\beta_x = \beta_y$  diagonal, as illustrated in Fig. 27.

## XIII. RECTANGULAR GRID MOTION

Consider a system of points tagged by the double indices  $i, j$ ;

$$x_{i,j} = x(i,j,t); \quad (270a)$$

$$y_{i,j} = y(i,j,t). \quad (270b)$$

Figure 28 illustrates the grid formed by Eq. (270) at a given time  $t$ . The pair of numbers at each point indicates  $(i,j)$ . For a strictly rectangular grid at all times (which includes Lagrangian grid motion),

$$x_{i,j} = x(i,t); \quad (271a)$$

$$y_{i,j} = y(j,t). \quad (271b)$$

which we therefore denote from now on by

$$x_i = x(i,t); \quad (272a)$$

$$y_j = y(j,t). \quad (272b)$$

This leads to a mesh as in Fig. 29.

#### XIV. GEOMETRICAL ASPECTS

We consider seven geometries. (These by no means cover the whole spectrum of two-dimensional systems.) In cartesian geometry, we have x-y (x-z or y-z); in cylindrical geometry, r-z, r- $\phi$ , and z- $\phi$ , and finally in spherical geometry r- $\theta$ , r- $\phi$ , and  $\theta$ - $\phi$ . Figure 30 illustrates a finite control volume in each of the different cases.

As explained earlier, when the grid moves the control surface area in the integral form of the conservation equations should be an average surface area defined as

$$\int_{S^{\text{mean}}} (\vec{u}^g \delta t \cdot \vec{n}) dS = \text{swept volume}.$$

In one-dimensional cases, the above definition reduces to defining  $A_{\text{interface}} = \frac{\text{swept volume}}{u^g \delta t}$ . In two dimensions, however, this is not enough. We have to find a path between the old grid and the new one such that we can construct a mean cell having its surfaces equal to the average areas and corners located on the above path.

##### 1. Cartesian Coordinates

Figure 31 illustrates the location of cell (i,j) at times  $t^n$  and  $t^{n+1} = t^n + \delta t$ . The left and right interfaces are denoted by  $(i - 1/2, j)$ ,  $(i, j + 1/2, j)$ , respectively, and the bottom and top ones by  $(i, j - 1/2)$ ,  $(i, j + 1/2)$ . We notice here that since all  $i \pm 1/2, j$  interfaces (different j's) move as a whole, the grid velocity is independent of j. It is therefore denoted by  $u_{i \pm 1/2}^g$  without a j index. The same is true for  $v_{j \pm 1/2}^g$ .

In cartesian geometry, it is obvious that the path needed is a straight line between the new and old corners of the cell, and the mean cell is halfway between the old cell and the new one.

The volume swept by interface  $(i \pm 1/2, j)$  is given by the product (average base)  $\times$  (height):

$$\begin{aligned}\Delta V_{i\pm\frac{1}{2},j} &= \frac{(y_{j+\frac{1}{2}}^n - y_{j-\frac{1}{2}}^n) + (y_{j+\frac{1}{2}}^{n+1} - y_{j-\frac{1}{2}}^{n+1})}{2} [x_{i\pm\frac{1}{2}}^{n+1} - x_{i\pm\frac{1}{2}}^n] \\ &= \frac{1}{2}(A_j^n + A_j^{n+1})^2 (x_{i\pm\frac{1}{2}}^{n+1} - x_{i\pm\frac{1}{2}}^n),\end{aligned}$$

where we notice again that the  $i$  index is omitted from  $A_{i\pm\frac{1}{2},j}$  since all the  $A_{i\pm\frac{1}{2},j}$  interfaces (different  $i$ 's) are equal. The above equation can be written as

$$\Delta V_{i\pm\frac{1}{2},j} = \left[ \left( \frac{y_{j+\frac{1}{2}}^n + y_{j+\frac{1}{2}}^{n+1}}{2} \right) - \left( \frac{y_{j-\frac{1}{2}}^n + y_{j-\frac{1}{2}}^{n+1}}{2} \right) \right] (x_{i\pm\frac{1}{2}}^{n+1} - x_{i\pm\frac{1}{2}}^n) \quad (286)$$

showing that the mean area is halfway between old and new. The grid velocity  $u_{i\pm\frac{1}{2}}^g$  in this case is considered constant,

$$u_{i\pm\frac{1}{2}}^g = \frac{x_{i\pm\frac{1}{2}}^{n+1} - x_{i\pm\frac{1}{2}}^n}{\delta t}, \quad (287)$$

and the mean area is

$$A_j^{n+\frac{1}{2}} = y_{j+\frac{1}{2}}^{n+\frac{1}{2}} - y_{j-\frac{1}{2}}^{n+\frac{1}{2}} = \frac{A_j^n + A_j^{n+1}}{2}, \quad (288a)$$

where

$$y_{j\pm\frac{1}{2}}^{n+\frac{1}{2}} = \frac{1}{2}(y_{j\pm\frac{1}{2}}^n + y_{j\pm\frac{1}{2}}^{n+1}). \quad (288b)$$

Similarly,

$$A_i^{n+1/2} = x_{i+1/2}^{n+1/2} - x_{i-1/2}^{n+1/2} = \frac{A_i^n + A_i^{n+1}}{2}, \quad (289a)$$

where

$$x_{i\pm 1/2}^{n+1/2} = \frac{1}{2}(x_{i\pm 1/2}^n + x_{i\pm 1/2}^{n+1}). \quad (289b)$$

The mean cell volume is

$$\psi_{i,j}^{n+1/2} = (y_{j+1/2}^{n+1/2} - y_{j-1/2}^{n+1/2})(x_{i+1/2}^{n+1/2} - x_{i-1/2}^{n+1/2}). \quad (290)$$

## 2. Cylindrical (r-z) Coordinates

Let us derive the required path between the corners of old and new cells such that the corners of the mean cell fall on that path. Figure 32 illustrates the old and new cells. Figure 33 shows the volume swept by interface  $(i, j \pm 1/2)$ :

$$\psi_{i,j\pm 1/2} = \int_{z_{j\pm 1/2}^n}^{z_{j\pm 1/2}^{n+1}} \pi r_{i\pm 1/2}^2 dz_{j\pm 1/2} - \int_{z_{j\pm 1/2}^n}^{z_{j\pm 1/2}^{n+1}} \pi r_{i-1/2}^2 dz_{j\pm 1/2}, \quad (291)$$

where it is obvious that a linear average can be obtained if  $r_{i\pm 1/2}^2$  is assumed to be linear in  $z_{j\pm 1/2}$ . Let

$$\frac{(r_{i\pm 1/2}^2)^2 - (r_{i\pm 1/2}^n)^2}{(r_{i\pm 1/2}^{n+1})^2 - (r_{i\pm 1/2}^n)^2} = \frac{z_{j\pm 1/2} - z_{j\pm 1/2}^n}{z_{j\pm 1/2}^{n+1} - z_{j\pm 1/2}^n}, \quad (292a)$$

i.e., a parabolic path. The above formula can be written concisely as

$$\frac{\Delta r_{i\pm 1/2}^2}{\Delta R_{i\pm 1/2}^2} = \frac{\Delta z_{j\pm 1/2}}{\Delta Z_{j\pm 1/2}}, \quad (292b)$$



yielding

$$r_{i+\frac{1}{2}}^2 = (r_{i+\frac{1}{2}}^n)^2 + \frac{\Delta z_{j+\frac{1}{2}}}{\Delta Z_{j+\frac{1}{2}}} \Delta R_{i+\frac{1}{2}}^2. \quad (292c)$$

Substituting (292c) into (291), we get

$$\begin{aligned} \Delta \Psi_{i,j+\frac{1}{2}} &= \pi \Delta Z_{j+\frac{1}{2}} \int_0^1 (r_{i+\frac{1}{2}}^2 - r_{i-\frac{1}{2}}^2) d\left(\frac{\Delta z_{j+\frac{1}{2}}}{\Delta Z_{j+\frac{1}{2}}}\right) \\ &= \pi \Delta Z_{j+\frac{1}{2}} \left[ \frac{(r_{i+\frac{1}{2}}^n)^2 + (r_{i+\frac{1}{2}}^{n+1})^2}{2} + \frac{(r_{i-\frac{1}{2}}^n)^2 + (r_{i-\frac{1}{2}}^{n+1})^2}{2} \right], \end{aligned}$$

yielding a mean area

$$A_i^{n+\frac{1}{2}} = \frac{\Delta \Psi_{i,j+\frac{1}{2}}}{\Delta Z_{j+\frac{1}{2}}} = \pi [(r_{i+\frac{1}{2}}^{n+\frac{1}{2}})^2 - (r_{i-\frac{1}{2}}^{n+\frac{1}{2}})^2] = \frac{A_i^n + A_i^{n+1}}{2}, \quad (293a)$$

where

$$r_{i+\frac{1}{2}}^{n+\frac{1}{2}} = \left( \frac{(r_{i+\frac{1}{2}}^n)^2 + (r_{i+\frac{1}{2}}^{n+1})^2}{2} \right)^{\frac{1}{2}} \quad (293b)$$

This shows the advantage of the parabolic path (292a), namely

$$\frac{\Delta z_{j+\frac{1}{2}}}{\Delta Z_{j+\frac{1}{2}}} = \frac{\Delta r_{i+\frac{1}{2}}^2}{\Delta R_{i+\frac{1}{2}}^2} = 1/2, \quad (293c)$$

i.e., the average area  $A_i^{n+\frac{1}{2}}$  is halfway along  $z$  between the old and new ones,

at

$$z_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{z_{j+\frac{1}{2}}^n + z_{j+\frac{1}{2}}^{n+1}}{2}. \quad (293d)$$

Following the nomenclature of Fig. 34, the volume swept by the inter-face  $i+\frac{1}{2}, j$  is

$$\begin{aligned}
\Delta \Psi_{i+\frac{1}{2},j} &= \int_{r_{i+\frac{1}{2}}^n}^{r_{i+\frac{1}{2}}^{n+1}} 2\pi r_{i+\frac{1}{2}} (z_{j+\frac{1}{2}} - z_{j-\frac{1}{2}}) dr_{i+\frac{1}{2}} \\
&= \int_{r_{i+\frac{1}{2}}^n}^{r_{i+\frac{1}{2}}^{n+1}} \pi (z_{j+\frac{1}{2}} - z_{j-\frac{1}{2}}) dr_{i+\frac{1}{2}}^2.
\end{aligned} \tag{294}$$

But

$$z_{j\pm\frac{1}{2}} = z_{j\pm\frac{1}{2}}^n + \Delta z_{j\pm\frac{1}{2}}, \tag{295}$$

yielding

$$\Delta \Psi_{i+\frac{1}{2},j} = \int_{r_{i+\frac{1}{2}}^n}^{r_{i+\frac{1}{2}}^{n+1}} \pi \left[ (z_{j+\frac{1}{2}}^n - z_{j-\frac{1}{2}}^n) + \left( \frac{\Delta z_{j+\frac{1}{2}}}{\Delta z_{j+\frac{1}{2}}} \Delta z_{j+\frac{1}{2}} - \frac{\Delta z_{j-\frac{1}{2}}}{\Delta z_{j-\frac{1}{2}}} \Delta z_{j-\frac{1}{2}} \right) \right] dr_{i+\frac{1}{2}}^2$$

which, with (292b) gives

$$\begin{aligned}
\Delta \Psi_{i+\frac{1}{2},j} &= \pi \Delta R_{i+\frac{1}{2}}^2 \int_0^1 [(z_{j+\frac{1}{2}}^n - z_{j-\frac{1}{2}}^n) \\
&\quad + \frac{\Delta r_{i+\frac{1}{2}}^2}{\Delta R_{i+\frac{1}{2}}^2} (\Delta z_{j+\frac{1}{2}} - \Delta z_{j-\frac{1}{2}})] d \frac{\Delta r_{i+\frac{1}{2}}^2}{\Delta R_{i+\frac{1}{2}}^2} \\
&= \pi \Delta R_{i+\frac{1}{2}}^2 [z_{j+\frac{1}{2}}^{n+\frac{1}{2}} + z_{j-\frac{1}{2}}^{n+\frac{1}{2}}].
\end{aligned} \tag{296}$$

Now to be able to construct a rectangular mean cell with its four corners on the parabolic paths of Eq. (292a), the quantities  $A_{i+\frac{1}{2},j}^{n+\frac{1}{2}}$  have to be also half way between old and new, i.e.,

$$A_{i\pm\frac{1}{2},j}^{n+\frac{1}{2}} = 2\pi r_{i\pm\frac{1}{2}}^{n+\frac{1}{2}} [z_{j+\frac{1}{2}}^{n+\frac{1}{2}} - z_{j-\frac{1}{2}}^{n+\frac{1}{2}}], \quad (297)$$

where we notice that the interface area is dependent on both  $i, j$ , in contrast to the cartesian case. With Eq. (296), Eq. (297) yields

$$A_{i\pm\frac{1}{2},j}^{n+\frac{1}{2}} = \frac{\Delta V_{i\pm\frac{1}{2}}}{\Delta R_{i\pm\frac{1}{2}}^2 / 2r_{i\pm\frac{1}{2}}^{n+\frac{1}{2}}} \quad (298)$$

whence, if  $u_{i\pm\frac{1}{2}}^g$  denotes the average velocity of the grid during  $t$ ,

$$u_{i\pm\frac{1}{2}}^g \delta t = \frac{(r_{i\pm\frac{1}{2}}^{n+1})^2 - (r_{i\pm\frac{1}{2}}^n)^2}{2r_{i\pm\frac{1}{2}}^{n+\frac{1}{2}}} \quad (299)$$

where, as is clear from Eq. (293a), it was assumed that

$$v_{j\pm\frac{1}{2}}^g \delta t = \Delta z_{j\pm\frac{1}{2}} = z_{j\pm\frac{1}{2}}^{n+1} - z_{j\pm\frac{1}{2}}^n. \quad (300)$$

The difference between the form of (299) and that of (300) is attributed to the parabolic path of the corner. If the grid velocity  $v_{j\pm\frac{1}{2}}^g$  is a constant during  $\delta t$ , we evaluate  $u_{i\pm\frac{1}{2}}^g$  at  $t^{n+\frac{1}{2}} = t^n + \frac{\delta t}{2}$  from (292c)

$$2r_{i\pm\frac{1}{2}} \frac{dr_{i\pm\frac{1}{2}}}{dt} = \frac{\Delta R_{i\pm\frac{1}{2}}^2}{\Delta z_{j\pm\frac{1}{2}}} \frac{d\Delta z_{j\pm\frac{1}{2}}}{dt} = \frac{\Delta R_{i\pm\frac{1}{2}}^2}{\Delta z_{j\pm\frac{1}{2}}} \frac{dz_{j\pm\frac{1}{2}}}{dt},$$

whence

$$u_{i\pm\frac{1}{2}}^g = \frac{\Delta R_{i\pm\frac{1}{2}}^2}{2r_{i\pm\frac{1}{2}}} \frac{v_{j\pm\frac{1}{2}}^g}{\Delta z_{j\pm\frac{1}{2}}} = \frac{\Delta R_{i\pm\frac{1}{2}}^2}{2r_{i\pm\frac{1}{2}} \delta t}, \quad (301)$$

using Eq. (300). Since  $v_{j\pm\frac{1}{2}}^g = \text{const.}$ ,  $(\Delta z_{j\pm\frac{1}{2}} / \Delta z_{j\pm\frac{1}{2}})_{t + \frac{\delta t}{2}} = 1/2$ .

Consequently, from (292c)

$$r_{i\pm\frac{1}{2}}^2 \Big|_{t + \frac{\delta t}{2}} = \frac{1}{2} [(r_{i\pm\frac{1}{2}}^n)^2 + (r_{i\pm\frac{1}{2}}^{n+1})^2] = (r_{i\pm\frac{1}{2}}^{n+\frac{1}{2}})^2,$$

thus reproducing Eq. (299) when substituted in Eq. (301). A more general definition of the average interface is therefore

$$\left[ \begin{array}{c} \text{mean} \\ \text{interface} \\ \text{area} \end{array} \right] = \frac{\text{swept volume}}{(\text{velocity of interface at } t^n + \frac{\delta t}{2}) \cdot \delta t} \quad (302)$$

where the denominator is approximately but not quite exactly equal to the distance the interface is shifted. Finally, the mean cell volume is

$$V_{i,j}^{n+1/2} = \pi [(r_{i+1/2}^{n+1/2})^2 - (r_{i-1/2}^{n+1/2})^2] [z_{j+1/2}^{n+1/2} - z_{j-1/2}^{n+1/2}]. \quad (303)$$

### 3. Spherical $r$ - $\theta$ Coordinates

Figure 35 illustrates cell  $i, j$  at  $t^n$  and  $t^{n+1}$ . Consider Fig. 36 showing the motion of interface  $i, j \pm 1/2$ . The volume swept by interface  $i, j \pm 1/2$  is

$$\begin{aligned} \Delta V_{i,j \pm 1/2} &= \int_{\theta_{j \pm 1/2}^n}^{\theta_{j \pm 1/2}^{n+1}} \frac{2\pi}{3} (r_{i+1/2}^3 - r_{i-1/2}^3) \sin \theta_{j \pm 1/2} d\theta_{j \pm 1/2} \\ &= \int_{\theta_{j \pm 1/2}^n}^{\theta_{j \pm 1/2}^{n+1}} \frac{2\pi}{3} (r_{i+1/2}^3 - r_{i-1/2}^3) d(-\cos \theta_{j \pm 1/2}), \end{aligned} \quad (304)$$

showing that we can get a linear average if  $r_{i \pm 1/2}^3$  is assumed to be a linear function of  $(-\cos \theta_{j \pm 1/2})$ . Let

$$\frac{(r_{i+1/2}^{n+1/2})^3 - (r_{i+1/2}^n)^3}{(r_{i-1/2}^{n+1/2})^3 - (r_{i-1/2}^n)^3} = \frac{\cos \theta_{j \pm 1/2}^n - \cos \theta_{j \pm 1/2}^{n+1/2}}{\cos \theta_{j \pm 1/2}^n - \cos \theta_{j \pm 1/2}^{n+1}}, \quad (305a)$$

or in a more concise form,

$$\frac{\Delta r_{i\pm\frac{1}{2}}^3}{\Delta R_{i\pm\frac{1}{2}}^3} = \frac{\Delta(-\cos \theta_{j\pm\frac{1}{2}})}{\Delta(-\cos \theta_{j\pm\frac{1}{2}})} \quad (305b)$$

This yields

$$r_{i\pm\frac{1}{2}}^3 = (r_{i\pm\frac{1}{2}}^n)^3 + \frac{\Delta(-\cos \theta_{j\pm\frac{1}{2}})}{\Delta(-\cos \theta_{j\pm\frac{1}{2}})} \Delta R_{i\pm\frac{1}{2}}^3 \quad (305c)$$

Substituting into Eq. (304) we get

$$\begin{aligned} \Delta \Psi_{i,j\pm\frac{1}{2}} &= \frac{2\pi}{3} \Delta(-\cos \theta_{j\pm\frac{1}{2}}) \int_0^1 [(r_{i\pm\frac{1}{2}}^{n3} - r_{i-\frac{1}{2}}^{n3}) \\ &\quad + \frac{\Delta(-\cos \theta_{j\pm\frac{1}{2}})}{\Delta(-\cos \theta_{j\pm\frac{1}{2}})} (\Delta R_{i\pm\frac{1}{2}}^3 - \Delta R_{i-\frac{1}{2}}^3)] d \frac{\Delta(-\cos \theta_{j\pm\frac{1}{2}})}{\Delta(-\cos \theta_{j\pm\frac{1}{2}})} \\ &= \frac{2\pi}{3} (\cos \theta_{j\pm\frac{1}{2}}^n - \cos \theta_{j\pm\frac{1}{2}}^{n+1}) \left[ \frac{(r_{i\pm\frac{1}{2}}^n)^3 + (r_{i\pm\frac{1}{2}}^{n+1})^3}{2} \right. \\ &\quad \left. - \frac{(r_{i-\frac{1}{2}}^n)^3 + (r_{i-\frac{1}{2}}^{n+1})^3}{2} \right]. \end{aligned} \quad (306)$$

We notice that the mean interface  $i, j\pm\frac{1}{2}$  is halfway on a cosine scale between

$\theta_{j\pm\frac{1}{2}}^n, \theta_{j\pm\frac{1}{2}}^{n+1}$  or on a cubic scale between  $r_{i\pm\frac{1}{2}}^n, r_{i\pm\frac{1}{2}}^{n+1}$ . As for interface

$(i\pm\frac{1}{2}, j)$ , it sweeps a volume (see Fig. 37),

$$\begin{aligned} \Delta \Psi_{i\pm\frac{1}{2},j} &= \int_{r_{i\pm\frac{1}{2}}^n}^{r_{i\pm\frac{1}{2}}^{n+1}} 2\pi r_{i\pm\frac{1}{2}}^2 (\cos \theta_{j-\frac{1}{2}} - \cos \theta_{j+\frac{1}{2}}) dr_{i\pm\frac{1}{2}} \\ &= \int_{r_{i\pm\frac{1}{2}}^n}^{r_{i\pm\frac{1}{2}}^{n+1}} \frac{2\pi}{3} (\cos \theta_{j-\frac{1}{2}} - \cos \theta_{j+\frac{1}{2}}) dr_{i\pm\frac{1}{2}}^3 \end{aligned} \quad (307)$$

But  $\cos \theta_{j\pm\frac{1}{2}} = \cos \theta_{j\pm\frac{1}{2}}^n + \Delta(-\cos \theta_{j\pm\frac{1}{2}})$ , yielding

$$\Delta\psi_{i\pm\frac{1}{2},j} = \frac{2\pi}{3} \int_{r_{i\pm\frac{1}{2}}^n}^{r_{i\pm\frac{1}{2}}^{n+1}} [(\cos \theta_{j-\frac{1}{2}}^n - \cos \theta_{j+\frac{1}{2}}^n) + \frac{\Delta(-\cos \theta_{j\pm\frac{1}{2}})}{\Delta(-\cos \theta_{j\pm\frac{1}{2}})} \{ \Delta(-\cos \theta_{j-\frac{1}{2}}) - \Delta(-\cos \theta_{j+\frac{1}{2}}) \}] dr_{i\pm\frac{1}{2}}^3,$$

which with Eq. (305b) results in

$$\begin{aligned} \Delta\psi_{i\pm\frac{1}{2},j} &= \frac{2\pi}{3} \Delta R_{i\pm\frac{1}{2}}^3 \int_0^1 [(\cos \theta_{j-\frac{1}{2}}^n - \cos \theta_{j+\frac{1}{2}}^{n+1}) \\ &\quad + \frac{\Delta r_{i\pm\frac{1}{2}}^3}{\Delta R_{i\pm\frac{1}{2}}^3} \{ \Delta(-\cos \theta_{j-\frac{1}{2}}) - \Delta(-\cos \theta_{j+\frac{1}{2}}) \}] d \frac{\Delta r_{i\pm\frac{1}{2}}^3}{\Delta R_{i\pm\frac{1}{2}}^3} \\ &= \frac{2\pi}{3} \Delta R_{i\pm\frac{1}{2}}^3 \left[ \frac{\cos \theta_{j-\frac{1}{2}}^n + \cos \theta_{j-\frac{1}{2}}^{n+1}}{2} - \frac{\cos \theta_{j+\frac{1}{2}}^n + \cos \theta_{j+\frac{1}{2}}^{n+1}}{2} \right]. \quad (308) \end{aligned}$$

Here we notice that interface  $i\pm\frac{1}{2},j$  is halfway on a cubic scale between  $r_{i\pm\frac{1}{2}}^n, r_{i\pm\frac{1}{2}}^{n+1}$  or on a cosine scale between  $\theta_{j\pm\frac{1}{2}}^n, \theta_{j\pm\frac{1}{2}}^{n+1}$ . Consequently, we can construct a mean cell having its corners on the paths of Eq. (305a). Let

$$r_{i\pm\frac{1}{2}}^{n+\frac{1}{2}} \equiv \left( \frac{(r_{i\pm\frac{1}{2}}^n)^3 + (r_{i\pm\frac{1}{2}}^{n+1})^3}{2} \right)^{1/3} \quad (309)$$

and

$$\cos \theta_{j\pm\frac{1}{2}}^{n+\frac{1}{2}} \equiv \frac{\cos \theta_{j\pm\frac{1}{2}}^n + \cos \theta_{j\pm\frac{1}{2}}^{n+1}}{2}. \quad (310)$$

Eqs. (306) and (308) can be written then as

$$\Delta\psi_{i,j\pm\frac{1}{2}} = \frac{2\pi}{3} (\cos \theta_{j\pm\frac{1}{2}}^n - \cos \theta_{j\pm\frac{1}{2}}^{n+1}) [(r_{i\pm\frac{1}{2}}^{n+\frac{1}{2}})^3 - (r_{i-\frac{1}{2}}^{n+\frac{1}{2}})^3] \quad (311)$$

and

$$\Delta\psi_{i\pm\frac{1}{2},j} = \frac{2\pi}{3} (\cos \theta_{j-\frac{1}{2}}^{n+\frac{1}{2}} - \cos \theta_{j+\frac{1}{2}}^{n+\frac{1}{2}}) [(r_{i\pm\frac{1}{2}}^{n+1})^3 - (r_{i\pm\frac{1}{2}}^n)^3], \quad (312)$$

respectively. Now in order to be able to construct the average cell,  $A_{i,j\pm\frac{1}{2}}$  and  $A_{i\pm\frac{1}{2},j}$  should take the forms

$$A_{i,j\pm\frac{1}{2}}^{n+\frac{1}{2}} = \pi [(r_{i\pm\frac{1}{2}}^{n+\frac{1}{2}})^2 - (r_{i-\frac{1}{2}}^{n+\frac{1}{2}})^2] \sin \theta_{j\pm\frac{1}{2}}^{n+\frac{1}{2}}, \quad (313a)$$

forcing the choice

$$v_{i,j\pm\frac{1}{2}}^g \delta t = \frac{\Delta\psi_{i,j\pm\frac{1}{2}}}{A_{i,j\pm\frac{1}{2}}^{n+\frac{1}{2}}} = \frac{2}{3} \frac{(r_{i\pm\frac{1}{2}}^{n+\frac{1}{2}})^3 - (r_{i-\frac{1}{2}}^{n+\frac{1}{2}})^3}{(r_{i\pm\frac{1}{2}}^{n+\frac{1}{2}})^2 - (r_{i-\frac{1}{2}}^{n+\frac{1}{2}})^2} \frac{\cos \theta_{j\pm\frac{1}{2}}^n - \cos \theta_{j\pm\frac{1}{2}}^{n+1}}{\sin \theta_{j\pm\frac{1}{2}}^{n+\frac{1}{2}}}, \quad (313b)$$

and

$$A_{i\pm\frac{1}{2},j}^{n+\frac{1}{2}} = 2\pi (r_{i\pm\frac{1}{2}}^{n+\frac{1}{2}})^2 (\cos \theta_{j-\frac{1}{2}}^{n+\frac{1}{2}} - \cos \theta_{j+\frac{1}{2}}^{n+\frac{1}{2}}), \quad (314a)$$

forcing the choice

$$u_{i\pm\frac{1}{2}}^g \delta t = \frac{\Delta\psi_{i\pm\frac{1}{2},j}}{A_{i\pm\frac{1}{2},j}^{n+\frac{1}{2}}} = \frac{(r_{i\pm\frac{1}{2}}^{n+1})^3 - (r_{i\pm\frac{1}{2}}^n)^3}{3(r_{i\pm\frac{1}{2}}^{n+\frac{1}{2}})^2}. \quad (314b)$$

To complete the formulation, it remains to check the consistency of the two velocities  $u_{i\pm\frac{1}{2}}^g$ ,  $v_{i,j\pm\frac{1}{2}}^g$ , namely that they occur at the same instant.

Differentiating (305a) with respect to time and taking  $r_{i\pm\frac{1}{2}}^n$ ,  $\theta_{j\pm\frac{1}{2}}^n$  at the moment when they are halfway i.e.,  $r_{i\pm\frac{1}{2}}^{n+\frac{1}{2}}$ ,  $\theta_{j\pm\frac{1}{2}}^{n+\frac{1}{2}}$ , we get

$$\frac{3(r_{i\pm\frac{1}{2}}^{n+\frac{1}{2}})^2 (dr_{i\pm\frac{1}{2}}/dt)^{n+\frac{1}{2}}}{(r_{i\pm\frac{1}{2}}^{n+1})^3 - (r_{i\pm\frac{1}{2}}^n)^3} = \frac{\sin \theta_{j\pm\frac{1}{2}}^{n+1} (d\theta_{j\pm\frac{1}{2}}/dt)^{n+\frac{1}{2}}}{\cos \theta_{j\pm\frac{1}{2}}^n - \cos \theta_{j\pm\frac{1}{2}}^{n+1}}.$$

Recognizing that  $(dr_{i\pm\frac{1}{2}}/dt)^{n+\frac{1}{2}} = u_{i\pm\frac{1}{2}}^g$ , the velocity of the grid at  $t^n + \frac{\delta t}{2}$ , from Eq. (314b) and the above equation we obtain

$$\left( \frac{d\theta_{j\pm\frac{1}{2}}}{dt} \right)^{n+\frac{1}{2}} \delta t = \frac{\cos \theta_{j\pm\frac{1}{2}}^n - \cos \theta_{j\pm\frac{1}{2}}^{n+1}}{\sin \theta_{j\pm\frac{1}{2}}^{n+\frac{1}{2}}}, \quad (315)$$

whence from Eq. (313b), the velocity of the grid at  $t^n + \frac{\delta t}{2}$ ,

$$v_{i,j\pm\frac{1}{2}}^g = \frac{2}{3} \frac{(r_{i+\frac{1}{2}}^{n+\frac{1}{2}})^3 - (r_{i-\frac{1}{2}}^{n+\frac{1}{2}})^3}{(r_{i+\frac{1}{2}}^{n+\frac{1}{2}})^2 - (r_{i-\frac{1}{2}}^{n+\frac{1}{2}})^2} \left(\frac{d\vartheta_{j\pm\frac{1}{2}}}{dt}\right)^{n+\frac{1}{2}} \quad (316)$$

Recognizing  $\left(\frac{d\vartheta_{j\pm\frac{1}{2}}}{dt}\right)$  as the angular velocity at  $t^n + \delta t/2$  of the interface  $i, j\pm\frac{1}{2}$  [from Eq. (315) obviously independent of index  $i$  as expected after the discussion in the section "Rectangular Grid Motion"], we can define an average radius for the interface  $i, j\pm\frac{1}{2}$  (independent of  $j$ ) as

$$R_i^{n+\frac{1}{2}} = \frac{\frac{1}{3}[(r_{i+\frac{1}{2}}^{n+\frac{1}{2}})^2 + (r_{i+\frac{1}{2}}^{n+\frac{1}{2}})(r_{i-\frac{1}{2}}^{n+\frac{1}{2}}) + (r_{i-\frac{1}{2}}^{n+\frac{1}{2}})^2]}{\frac{1}{2}[(r_{i+\frac{1}{2}}^{n+\frac{1}{2}}) + (r_{i-\frac{1}{2}}^{n+\frac{1}{2}})]} \quad (317)$$

Finally, the mean cell volume is

$$\bar{v}_{i,j}^{n+\frac{1}{2}} = \frac{2\pi}{3} [(r_{i+\frac{1}{2}}^{n+\frac{1}{2}})^3 - (r_{i-\frac{1}{2}}^{n+\frac{1}{2}})^3] (\cos \vartheta_{j-\frac{1}{2}}^{n+\frac{1}{2}} - \cos \vartheta_{j+\frac{1}{2}}^{n+\frac{1}{2}}). \quad (318)$$

Coordinate cases 4-7 will be treated in a later report.



## XV. SOURCE TERMS

As explained earlier, source terms are integrated either over cell volume or over cell interface area. The volumes and areas used are those of the mean cell. The balance of source terms is the main reason for the necessity of a closed mean cell construction, i.e., the ability to construct a closed cell whose corners are on the paths between old and new cell corners. For example, if we try to solve a hydrostatic pressure problem in cylindrical r-z coordinates, the momentum equation is nothing but the balance of the body gravity force and the pressure force on the top and bottom surfaces. If the mid-cell interfaces compose a closed surface enclosing the midway cell which happens to have a volume consistent with the interface areas, force balance is already guaranteed (provided the pressures are correct).

Let us consider the difference form of  $-\int_{sg} \vec{p} n ds$  (yielding  $-\text{grad } p$ ) in the three coordinate axes considered above. The resulting forces along the x, y directions are

$$F_{x_{i,j}} = (p_{i-\frac{1}{2},j}^{n+\frac{1}{2}} - p_{i+\frac{1}{2},j}^{n+\frac{1}{2}}) A_i^{n+\frac{1}{2}}; \quad (321a)$$

$$F_{y_{i,j}} = (p_{i,j-\frac{1}{2}}^{n+\frac{1}{2}} - p_{i,j+\frac{1}{2}}^{n+\frac{1}{2}}) A_j^{n+\frac{1}{2}}; \quad (321b)$$

respectively, where

$$p_{i+\frac{1}{2},j}^{n+\frac{1}{2}} = \frac{p_{i,j}^{n+\frac{1}{2}} + p_{i+1,j}^{n+\frac{1}{2}}}{2} \quad (322a)$$

and

$$p_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{p_{i,j}^{n+\frac{1}{2}} + p_{i,j+1}^{n+\frac{1}{2}}}{2}. \quad (322b)$$

In cylindrical r-z coordinates,

$$F_{r,i,j}^{n+\frac{1}{2}} = p_{i-\frac{1}{2},j}^{n+\frac{1}{2}} A_{i-\frac{1}{2},j}^{n+\frac{1}{2}} - p_{i+\frac{1}{2},j}^{n+\frac{1}{2}} A_{i+\frac{1}{2},j}^{n+\frac{1}{2}} + 2\pi p_{i,j}^{n+\frac{1}{2}} (r_{i+\frac{1}{2}}^{n+\frac{1}{2}} - r_{i-\frac{1}{2}}^{n+\frac{1}{2}}) (z_{j+\frac{1}{2}}^{n+\frac{1}{2}} - z_{j-\frac{1}{2}}^{n+\frac{1}{2}}),$$

which with Eq. (303) yields

$$F_{r,i,j}^{n+\frac{1}{2}} = p_{i-\frac{1}{2},j}^{n+\frac{1}{2}} A_{i-\frac{1}{2},j}^{n+\frac{1}{2}} - p_{i+\frac{1}{2},j}^{n+\frac{1}{2}} A_{i+\frac{1}{2},j}^{n+\frac{1}{2}} + \frac{p_{i,j}^{n+\frac{1}{2}} v_{i,j}^{n+\frac{1}{2}}}{r_i^{n+\frac{1}{2}}}, \quad (323a)$$

where

$$r_i^{n+\frac{1}{2}} = \frac{r_{i+\frac{1}{2}}^{n+\frac{1}{2}} + r_{i-\frac{1}{2}}^{n+\frac{1}{2}}}{2}. \quad (324)$$

We notice that  $p_{i,j}^{n+\frac{1}{2}}/r_i^{n+\frac{1}{2}}$  acts as a body force per unit volume. The force in the z-direction is

$$F_{z,i,j}^{n+\frac{1}{2}} = (p_{i,j-\frac{1}{2}}^{n+\frac{1}{2}} - p_{i,j+\frac{1}{2}}^{n+\frac{1}{2}}) A_i^{n+\frac{1}{2}}. \quad (323b)$$

In spherical r- $\theta$  coordinates, as illustrated in Fig. 38, the pressure acting on the hatched area creates a resultant force normal to the axis from which  $\theta$  is measured, which in turn gives rise to a radial component  $F_r'$  and a tangential component  $F_\theta'$ . This situation, namely, the creation of a body-force-like component, occurs whenever the area of parallel surfaces of the cell are not equal. This is bound to happen whenever the interface area depends on both indices i,j. A simple way to evaluate the force generated is the "pressure x projected area" since this area is the difference between the areas of these parallel surfaces. The radial force is therefore

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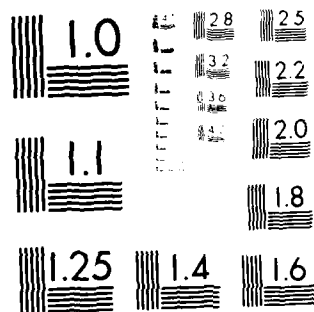
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$$F_{r_{i,j}} = p_{i-\frac{1}{2},j}^{n+\frac{1}{2}} A_{i-\frac{1}{2},j}^{n+\frac{1}{2}} - p_{i+\frac{1}{2},j}^{n+\frac{1}{2}} A_{i+\frac{1}{2},j}^{n+\frac{1}{2}} + F'_{r_{i,j}},$$

where

$$F'_{r_{i,j}} = p_{i,j}^{n+\frac{1}{2}} (A_{i+\frac{1}{2},j}^{n+\frac{1}{2}} - A_{i-\frac{1}{2},j}^{n+\frac{1}{2}}) = 2\pi p_{i,j}^{n+\frac{1}{2}} [(r_{i+\frac{1}{2}}^{n+\frac{1}{2}})^2 - (r_{i-\frac{1}{2}}^{n+\frac{1}{2}})^2] (\cos \theta_{j-\frac{1}{2}}^{n+\frac{1}{2}} - \cos \theta_{j+\frac{1}{2}}^{n+\frac{1}{2}}) = \frac{2p_{i,j}^{n+\frac{1}{2}} \psi_{i,j}^{n+\frac{1}{2}}}{R_i^{n+\frac{1}{2}}};$$

$R_i$  was defined earlier in Eq. (317). Thus

$$F_{r_{i,j}} = p_{i-\frac{1}{2},j}^{n+\frac{1}{2}} A_{i-\frac{1}{2},j}^{n+\frac{1}{2}} - p_{i+\frac{1}{2},j}^{n+\frac{1}{2}} A_{i+\frac{1}{2},j}^{n+\frac{1}{2}} + \frac{2p_{i,j}^{n+\frac{1}{2}} \psi_{i,j}^{n+\frac{1}{2}}}{R_i^{n+\frac{1}{2}}}. \quad (325)$$

As for the tangential direction,

$$F_{\theta_{i,j}} = p_{i,j-\frac{1}{2}}^{n+\frac{1}{2}} A_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} - p_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} A_{i,j-\frac{1}{2}}^{n+\frac{1}{2}} + F'_{\theta_{i,j}},$$

where

$$F'_{\theta_{i,j}} = p_{i,j}^{n+\frac{1}{2}} (A_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} - A_{i,j-\frac{1}{2}}^{n+\frac{1}{2}}) = \pi p_{i,j}^{n+\frac{1}{2}} [(r_{i+\frac{1}{2}}^{n+\frac{1}{2}})^2 - (r_{i-\frac{1}{2}}^{n+\frac{1}{2}})^2] (\sin \theta_{j+\frac{1}{2}}^{n+\frac{1}{2}} - \sin \theta_{j-\frac{1}{2}}^{n+\frac{1}{2}}).$$

If we note that

$$\sin \theta_{j+\frac{1}{2}}^{n+\frac{1}{2}} - \sin \theta_{j-\frac{1}{2}}^{n+\frac{1}{2}} = 2 \sin \left( \frac{\theta_{j+\frac{1}{2}}^{n+\frac{1}{2}} - \theta_{j-\frac{1}{2}}^{n+\frac{1}{2}}}{2} \right) \cos \left( \frac{\theta_{j+\frac{1}{2}}^{n+\frac{1}{2}} + \theta_{j-\frac{1}{2}}^{n+\frac{1}{2}}}{2} \right)$$

and

$$\cos \theta_{j-\frac{1}{2}}^{n+\frac{1}{2}} - \cos \theta_{j+\frac{1}{2}}^{n+\frac{1}{2}} = 2 \sin \left( \frac{\theta_{j+\frac{1}{2}}^{n+\frac{1}{2}} + \theta_{j-\frac{1}{2}}^{n+\frac{1}{2}}}{2} \right) \sin \left( \frac{\theta_{j+\frac{1}{2}}^{n+\frac{1}{2}} - \theta_{j-\frac{1}{2}}^{n+\frac{1}{2}}}{2} \right)$$

and using Eq. (318),  $F'_{\theta}$  can be expressed as

$$F_{i,j}^{n+1} = \frac{p_{i,j}^{n+1} v_{i,j}^{n+1}}{R_i^{n+1} \tan \theta_j^{n+1}},$$

where

$$\theta_j^{n+1} = \frac{\theta_{j+1}^{n+1} + \theta_{j-1}^{n+1}}{2}. \quad (326)$$

Thus

$$F_{i,j}^{n+1} = p_{i,j-1}^{n+1} A_{i,j-1}^{n+1} - p_{i,j+1}^{n+1} A_{i,j+1}^{n+1} + \frac{p_{i,j}^{n+1} v_{i,j}^{n+1}}{R_i^{n+1} \tan \theta_j^{n+1}},$$

Next, let us consider the difference form of  $-\int_{s_g} \vec{p} \cdot \vec{n} ds$  [yielding - div( $\vec{p}u$ )].

For the three coordinate systems considered above, the power added to the cell (i,j) is

$$\begin{aligned} P_{i,j} = & p_{i-1,j}^{n+1} u_{i-1,j}^{n+1} A_{i-1,j}^{n+1} - p_{i+1,j}^{n+1} u_{i+1,j}^{n+1} A_{i+1,j}^{n+1} \\ & + p_{i,j-1}^{n+1} v_{i,j-1}^{n+1} A_{i,j-1}^{n+1} - p_{i,j+1}^{n+1} v_{i,j+1}^{n+1} A_{i,j+1}^{n+1}, \end{aligned} \quad (328)$$

where

$$u_{i+1,j}^{n+1} = \frac{u_{i,j}^{n+1} + u_{i+1,j}^{n+1}}{2} \quad (329a)$$

and

$$v_{i,j+1}^{n+1} = \frac{v_{i,j}^{n+1} + v_{i,j+1}^{n+1}}{2}. \quad (329b)$$

The forces  $(F_x, F_y)$ ,  $(F_r, F_z)$ , and  $(F_r, F_\theta)$ , and the power  $P$  constitute a sample of the source terms encountered in treating generalized continuity equations. These are denoted by source  $_{i,j}^{n+1}$  in the next section.

## XVI. ALGORITHM

We describe the implementation of the scheme of Eqs. (223). The program and calling sequence are listed in the Appendix.

Assume a rectangular grid in two dimensions denoted by the coordinates  $x, y$  (not necessarily cartesian; for example  $x \equiv r, y \equiv \theta$  yield spherical coordinates). Let the interfaces coordinates be  $x_{1/2}, x_{3/2}, \dots, x_{N_x+1/2}; y_{1/2}, y_{3/2}, \dots, y_{N_y+1/2}$  (see Fig. 39).

The cell centers are located midway between the interfaces and are denoted by a pair of indices  $(i, j)$ , corresponding to  $(x, y)$ , respectively. The cell volumes are given by

$$V_{i,j}^{n,n+1} = \begin{cases} \text{cartesian} & : (y_{j+1/2}^{n,n+1} - y_{j-1/2}^{n,n+1})(x_{i+1/2}^{n,n+1} - x_{i-1/2}^{n,n+1}); \\ \text{cylindrical} & : [(x_{i+1/2}^{n,n+1})^2 - (x_{i-1/2}^{n,n+1})^2][y_{j+1/2}^{n,n+1} - y_{j-1/2}^{n,n+1}] \\ & \quad r-z \\ \text{spherical} & : \frac{2\pi}{3} [(x_{i+1/2}^{n,n+1})^3 - (x_{i-1/2}^{n,n+1})^3][\cos y_{j-1/2}^{n,n+1} - \cos y_{j+1/2}^{n,n+1}]; \\ & \quad r-\theta \end{cases}$$

We have then

$$\begin{aligned} \psi_{i,j}^{n+1} \rho_{i,j}^{T_x} &= \psi_{i,j}^n \rho_{i,j}^n - \delta t (\rho_{i+1/2,j}^n A_{i+1/2,j}^{n+1/2} \delta U_{i+1/2,j}^{n+1/2}) \\ &\quad + \delta t (\rho_{i-1/2,j}^n A_{i-1/2,j}^{n+1/2} \delta U_{i-1/2,j}^{n+1/2}) + \text{source}_{i,j}^{n+1/2} \end{aligned} \quad (332a)$$

and

$$\begin{aligned} \psi_{i,j}^{n+1} \rho_{i,j}^T = & \psi_{i,j}^n \rho_{i,j}^n - \delta t (\rho_{i,j+\frac{1}{2}}^n A_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} \delta V_{i,j+\frac{1}{2}}^{n+\frac{1}{2}}) \\ & + \delta t (\rho_{i,j-\frac{1}{2}}^n A_{i,j-\frac{1}{2}}^{n+\frac{1}{2}} \delta V_{i,j-\frac{1}{2}}^{n+\frac{1}{2}}) + \text{source}_{i,j}^{n+\frac{1}{2}} \end{aligned} \quad (332b)$$

for  $(i = 1, \dots, N_x)$  and  $(j = 1, \dots, N_y)$ , where

$$\rho_{i+\frac{1}{2},j}^n = \frac{\rho_{i,j}^n + \rho_{i+1,j}^n}{2} \quad (33a)$$

for  $i = 1, \dots, N_x - 1$  and  $j = 1, \dots, N_y$ , while

$$\rho_{i,j+\frac{1}{2}}^n = \frac{\rho_{i,j}^n + \rho_{i,j+1}^n}{2} \quad (33b)$$

for  $i = 1, \dots, N_x$  and  $j = 1, \dots, N_y - 1$ . The boundary values  $\rho_{\frac{1}{2},j}^n, \rho_{N_x+\frac{1}{2},j}^n$  are obtained from

$$\begin{aligned} \rho_{\frac{1}{2},j}^n &= \frac{\rho_{1,j}^n + \rho_{L,j}^n}{2}, \\ \rho_{N_x+\frac{1}{2},j}^n &= \frac{\rho_{N_x,j}^n + \rho_{R,j}^n}{2}, \end{aligned}$$

for  $(j = 1, \dots, N_y)$  where L and R denote left and right boundaries, respectively, while

$$\begin{aligned} \rho_{i,\frac{1}{2}}^n &= \frac{\rho_{i,1}^n + \rho_{i,B}^n}{2}, \\ \rho_{i,N_y+\frac{1}{2}}^n &= \frac{\rho_{i,N_y}^n + \rho_{i,T}^n}{2}, \end{aligned}$$

for  $(i = 1, \dots, N_x)$  where B and T denote bottom and top boundaries,



respectively. The mean interface areas  $A_{i+\frac{1}{2},j}^{n+\frac{1}{2}}$  and  $A_{i,j+\frac{1}{2}}^{n+\frac{1}{2}}$  are given by

$$A_{i+\frac{1}{2},j}^{n+\frac{1}{2}} = y_{j+\frac{1}{2}}^{n+\frac{1}{2}} - y_{j-\frac{1}{2}}^{n+\frac{1}{2}} \quad (334a)$$

and

$$A_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} = x_{i+\frac{1}{2}}^{n+\frac{1}{2}} - x_{i-\frac{1}{2}}^{n+\frac{1}{2}}, \quad (334b)$$

where

$$y_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{y_{j+\frac{1}{2}}^n + y_{j+\frac{1}{2}}^{n+1}}{2} \quad (335a)$$

and

$$x_{i+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{x_{i+\frac{1}{2}}^n + x_{i+\frac{1}{2}}^{n+1}}{2} \quad (335b)$$

for cartesian x-y coordinates; by

$$A_{i+\frac{1}{2},j}^{n+\frac{1}{2}} = 2\pi x_{i+\frac{1}{2}}^{n+\frac{1}{2}} (y_{j+\frac{1}{2}}^{n+\frac{1}{2}} - y_{j-\frac{1}{2}}^{n+\frac{1}{2}}) \quad (336a)$$

and

$$A_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} = \pi [(x_{i+\frac{1}{2}}^{n+\frac{1}{2}})^2 - (x_{i-\frac{1}{2}}^{n+\frac{1}{2}})^2], \quad (336b)$$

where

$$y_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{y_{j+\frac{1}{2}}^n + y_{j+\frac{1}{2}}^{n+1}}{2} \quad (337a)$$

and

$$x_{i+\frac{1}{2}}^{n+\frac{1}{2}} = \left[ \frac{(x_{i+\frac{1}{2}}^n)^2 + (x_{i+\frac{1}{2}}^{n+1})^2}{2} \right]^{\frac{1}{2}} \quad (337b)$$

for cylindrical r-z coordinates; and by

$$A_{i+\frac{1}{2},j}^{n+\frac{1}{2}} = 2\pi (x_{i+\frac{1}{2}}^{n+\frac{1}{2}})^2 [\cos y_{j-\frac{1}{2}}^{n+\frac{1}{2}} - \cos y_{j+\frac{1}{2}}^{n+\frac{1}{2}}] \quad (338a)$$

and

$$A_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} = \pi [x_{i+\frac{1}{2}}^{n+\frac{1}{2}}]^2 - (x_{i-\frac{1}{2}}^{n+\frac{1}{2}})^2] \sin y_{j+\frac{1}{2}}^{n+\frac{1}{2}}, \quad (338b)$$

where

$$y_{j+\frac{1}{2}}^{n+\frac{1}{2}} = \arccos \left[ \frac{1}{2} \{ \cos y_{j+\frac{1}{2}}^n + \cos y_{j+\frac{1}{2}}^{n+1} \} \right] \quad (339a)$$

and

$$x_{i+\frac{1}{2}}^{n+\frac{1}{2}} \left[ \frac{(x_{i+\frac{1}{2}}^n)^3 + (x_{i+\frac{1}{2}}^{n+1})^3}{2} \right]^{1/3} \quad (339b)$$

for spherical  $r-\theta$  coordinates. Finally,

$$\delta U_{i+\frac{1}{2},j}^{n+\frac{1}{2}} = u_{i+\frac{1}{2},j}^{n+\frac{1}{2}} - u_{i+\frac{1}{2},j}^g \quad (340a)$$

and

$$\delta V_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} = v_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} - v_{i,j+\frac{1}{2}}^g \quad (341a)$$

The grid velocities  $u_{i+\frac{1}{2},j}^g, v_{i,j+\frac{1}{2}}^g$  are given by

$$u_{i+\frac{1}{2},j}^g = \frac{x_{i+\frac{1}{2}}^{n+1} - x_{i+\frac{1}{2}}^n}{\delta t} \quad (341b)$$

$$v_{i,j+\frac{1}{2}}^g = \frac{y_{j+\frac{1}{2}}^{n+1} - y_{j+\frac{1}{2}}^n}{\delta t}$$

for cartesian  $x-y$  coordinates; by

$$u_{i+\frac{1}{2},j}^g = \frac{(x_{i+\frac{1}{2}}^{n+1})^2 - (x_{i+\frac{1}{2}}^n)^2}{2 x_{i+\frac{1}{2}}^{n+\frac{1}{2}} \delta t} \quad (342a)$$

$$v_{i,j+\frac{1}{2}}^g = \frac{y_{j+\frac{1}{2}}^{n+1} - y_{j+\frac{1}{2}}^n}{\delta t} \quad (342b)$$

for cylindrical r-z coordinates; and by

$$u_{i+\frac{1}{2},j}^g = \frac{(x_{i+\frac{1}{2}}^{n+1})^3 - (x_{i+\frac{1}{2}}^n)^3}{3(x_{i+\frac{1}{2}}^{n+1})^2 \delta t} \quad (343a)$$

$$v_{i,j+\frac{1}{2}}^g = \frac{x_i^{n+\frac{1}{2}}}{\delta t} \frac{\cos y_{j+\frac{1}{2}}^n - \cos y_{j+\frac{1}{2}}^{n+1}}{\sin y_{j+\frac{1}{2}}^{n+\frac{1}{2}}} \quad (343b)$$

for spherical r- $\theta$  coordinates, where

$$x_i^{n+\frac{1}{2}} = \frac{2}{3} \frac{(x_{i+\frac{1}{2}}^{n+\frac{1}{2}})^2 + (x_{i+\frac{1}{2}}^{n+\frac{1}{2}})(x_{i-\frac{1}{2}}^{n+\frac{1}{2}}) + (x_{i-\frac{1}{2}}^{n+\frac{1}{2}})^2}{x_{i+\frac{1}{2}}^{n+\frac{1}{2}} + x_{i-\frac{1}{2}}^{n+\frac{1}{2}}} \quad (344)$$

Equations (334)-(344) are valid for  $i = 0, 1, \dots, N_x$  and  $j = 0, 1, \dots, N_y$ .

Equations (332) yield  $\rho_{i,j}^{Tx}$  and  $\rho_{i,j}^{Ty}$ , which are used later to evaluate the antidiffusion fluxes. The transported and diffused densities are then obtained from

$$\begin{aligned} \psi_{i,j}^{n+1} \rho_{i,j}^{TD} &= \psi_{i,j}^{n+1} \rho_{i,j}^T + v_{i+\frac{1}{2},j} \psi_{i+\frac{1}{2},j}^{n+1} (\rho_{i+1,j}^n - \rho_{i,j}^n) \\ &\quad - v_{i-\frac{1}{2},j} \psi_{i-\frac{1}{2},j}^{n+1} (\rho_{i,j}^n - \rho_{i-1,j}^n) + v_{i,j+\frac{1}{2}} \psi_{i,j+\frac{1}{2}}^{n+1} (\rho_{i,j+1}^n \\ &\quad - \rho_{i,j}^n) - v_{i,j-\frac{1}{2}} \psi_{i,j-\frac{1}{2}}^{n+1} (\rho_{i,j}^n - \rho_{i,j-1}^n) \end{aligned} \quad (346)$$

for  $i = 1, \dots, N_x$  and  $j = 1, \dots, N_y$ , where

$$v_{i+\frac{1}{2},j} = \frac{1}{6} + \frac{1}{3} \epsilon_{i+\frac{1}{2},j}^2 \quad (347a)$$

and

$$v_{i,j+\frac{1}{2}} = \frac{1}{6} + \frac{1}{3} \varepsilon_{i,j+\frac{1}{2}}^2, \quad (347b)$$

while

$$v_{i+\frac{1}{2},j}^{n+1} = \frac{1}{2}(v_{i,j}^{n+1} + v_{i+1,j}^{n+1}) \quad (348a)$$

for  $i = 1, \dots, N_x - 1$  and  $j = 1, \dots, N_y$ . Similarly,

$$v_{i,j+\frac{1}{2}}^{n+1} = \frac{1}{2}(v_{i,j}^{n+1} + v_{i,j+1}^{n+1}) \quad (348b)$$

for  $i = 1, \dots, N_x$  and  $j = 1, \dots, N_y - 1$ . At the boundaries,

$$v_{\frac{1}{2},j}^{n+1} = v_{1,j}^{n+1} \quad \text{and} \quad v_{N_x+\frac{1}{2},j}^{n+1} = v_{N_x,j}^{n+1} \quad (349a)$$

for  $j = 1, \dots, N_y$ , while

$$v_{i,\frac{1}{2}}^{n+1} = v_{i,1}^{n+1} \quad \text{and} \quad v_{i,N_y+\frac{1}{2}}^{n+1} = v_{i,N_y}^{n+1} \quad (349b)$$

for  $i = 1, \dots, N_x$ . The dimensionless velocities  $\varepsilon_{i+\frac{1}{2},j}$ ,  $\varepsilon_{i,j+\frac{1}{2}}$  are obtained from

$$\varepsilon_{i+\frac{1}{2},j} = \frac{\delta U_{i+\frac{1}{2},j}^{n+\frac{1}{2}} A_{i+\frac{1}{2},j}^{n+\frac{1}{2}} \delta t}{2} \left( \frac{1}{v_{i,j}^{n+1}} + \frac{1}{v_{i+1,j}^{n+1}} \right) \quad (350a)$$

for  $i = 0, \dots, N_x$  and  $j = 1, \dots, N_y$  using (349a) and

$$\varepsilon_{i,j+\frac{1}{2}} = \frac{\delta V_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} A_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} \delta t}{2} \left( \frac{1}{v_{i,j}^{n+1}} + \frac{1}{v_{i,j+1}^{n+1}} \right) \quad (350b)$$

for  $i = 1, \dots, N_x$  and  $j = 0, \dots, N_y$  using (349b). The antidiffusion fluxes are then evaluated according to

$$F_{i+\frac{1}{2},j} = \mu_{i+\frac{1}{2},j} \psi_{i+\frac{1}{2},j}^{n+1} (\rho_{i+1,j}^{Tx} - \rho_{i,j}^{Tx}) \quad (351a)$$

and

$$F_{i,j+\frac{1}{2}} = \mu_{i,j+\frac{1}{2}} \psi_{i,j+\frac{1}{2}}^{n+1} (\rho_{i,j+1}^{Ty} - \rho_{i,j}^{Ty}), \quad (351b)$$

where

$$\mu_{i+\frac{1}{2},j} = \frac{1}{6} - \frac{2}{3} \epsilon_{i+\frac{1}{2},j}^2$$

and

$$\mu_{i,j+\frac{1}{2}} = \frac{1}{6} - \frac{2}{3} \epsilon_{i,j+\frac{1}{2}}^2.$$

## FLUX CORRECTION

The flux correction adopted here is that of Zalesak<sup>5</sup> in multi-dimensions. It "guarantees that the four antidiffusion fluxes, associated with each cell, acting in concert, do not create any ripples." In our notation it takes the following form:

1. A flux is cancelled if it is opposite to the local gradient of  $\rho^{TD}$  along the same direction, and if opposite to either or both adjacent gradients of  $\rho^{TD}$ , i.e.,  $F_{i+\frac{1}{2},j} = 0$  if

$$[F_{i+\frac{1}{2},j} (\rho_{i+1,j}^{TD} - \rho_{i,j}^{TD}) < 0] \text{ and } \{ [F_{i+\frac{1}{2},j} (\rho_{i+2,j}^{TD} - \rho_{i+1,j}^{TD}) < 0] \text{ or } [F_{i+\frac{1}{2},j} (\rho_{i,j}^{TD} - \rho_{i-1,j}^{TD}) < 0] \} \quad (352a)$$

and  $F_{i,j+\frac{1}{2}} = 0$  if

$$[F_{i,j+\frac{1}{2}}(\rho_{i,j+1}^{TD} - \rho_{i,j}^{TD}) < 0] \text{ and } \{[F_{i,j+\frac{1}{2}}(\rho_{i,j+2}^{TD} - \rho_{i,j+1}^{TD}) < 0] \text{ or } [F_{i,j+\frac{1}{2}}(\rho_{i,j}^{TD} - \rho_{i,j-1}^{TD}) < 0]\}. \quad (352b)$$

2. Evaluate the total in- and out-fluxes and their upper bounds.

Let  $P_{i,j}^+$  equal the sum of all antidiffusive fluxes "into" grid point  $(i,j)$ :

$$P_{i,j}^+ = \max(0, F_{i-\frac{1}{2},j}) - \min(0, F_{i+\frac{1}{2},j}) \\ + \max(0, F_{i,j-\frac{1}{2}}) - \min(0, F_{i,j+\frac{1}{2}}). \quad (353a)$$

Next we evaluate the upper bound  $Q_{i,j}^+$  on  $P_{i,j}^+$ :

$$Q_{i,j}^+ = (\rho_{i,j}^{\max} - \rho_{i,j}^{TD}) \Psi_{i,j}^{n+1}. \quad (354a)$$

The limiting ratio  $R_{i,j}^+$  is thus estimated as

$$R_{i,j}^+ = \begin{cases} \min(1, Q_{i,j}^+/P_{i,j}^+) & \text{if } P_{i,j}^+ > 0 \\ 0 & \text{if } P_{i,j}^+ = 0 \end{cases} \quad (355a)$$

Figure 40 illustrates the bounding process. Similarly, an upper bound  $Q_{i,j}^-$  is placed on the "outgoing" fluxes.

$$P_{i,j}^- = \max(0, F_{i+\frac{1}{2},j}) - \min(0, F_{i-\frac{1}{2},j}) \\ + \max(0, F_{i,j+\frac{1}{2}}) - \min(0, F_{i,j-\frac{1}{2}}) \quad (353b)$$

$$Q_{i,j}^- = (\rho_{i,j}^{TD} - \rho_{i,j}^{\min}) \Psi_{i,j}^{n+1} \quad (354b)$$

$$R_{i,j}^- = \begin{cases} \min(1, \frac{Q_{i,j}^-}{P_{i,j}^-}) & \text{if } P_{i,j}^- > 0 \\ 0 & \text{if } P_{i,j}^- = 0 \end{cases} \quad (355b)$$

In the above  $\rho_{i,j}^{\max}$ ,  $\rho_{i,j}^{\min}$  are the upper and lower bounds, respectively, on  $\rho_{i,j}^{n+1}$ , chosen so as to guarantee no ripples formation at grid point  $(i,j)$ . Finally, since each flux leaves a cell to enter an adjacent one,

3. The fluxes correction factors are defined as

$$C_{i+\frac{1}{2},j} = \begin{cases} \min (R_{i+\frac{1}{2},j}^+, R_{i,j}^-) & \text{if } F_{i+\frac{1}{2},j} \geq 0 \\ \min (R_{i+\frac{1}{2},j}^-, R_{i,j}^+) & \text{if } F_{i+\frac{1}{2},j} < 0 \end{cases} \quad (356a)$$

and

$$C_{i,j+\frac{1}{2}} = \begin{cases} \min (R_{i,j+\frac{1}{2}}^+, R_{i,j}^-) & \text{if } F_{i,j+\frac{1}{2}} \geq 0 \\ \min (R_{i,j+\frac{1}{2}}^-, R_{i,j}^+) & \text{if } F_{i,j+\frac{1}{2}} < 0. \end{cases} \quad (356b)$$

The corrected fluxes are given by

$$F_{i+\frac{1}{2},j}^C = C_{i+\frac{1}{2},j} F_{i+\frac{1}{2},j}, \quad (357a)$$

$$F_{i,j+\frac{1}{2}}^C = C_{i,j+\frac{1}{2}} F_{i,j+\frac{1}{2}}, \quad (357b)$$

4. For  $\rho_j^{\max}$  and  $\rho_j^{\min}$ , two choices are presented. A conservative choice would be

$$\rho_{i,j}^{\max} = \max (\rho_{i-1,j}^{TD}, \rho_{i,j-1}^{TL}, \rho_{i,j}^{TD}, \rho_{i+1,j}^{TD}, \rho_{i,j+1}^{TD}); \quad (358a)$$

$$\rho_{i,j}^{\min} = \min (\rho_{i-1,j}^{TD}, \rho_{i,j-1}^{TD}, \rho_{i,j}^{TD}, \rho_{i+1,j}^{TD}, \rho_{i,j+1}^{TD}). \quad (358b)$$

A more tolerant choice that gets rid of the problems of "clipping" and "terracing" partially is

$$\rho_{i,j}^{\max} = \max (\rho_{i-1,j}^a, \rho_{i,j-1}^a, \rho_{i,j}^a, \rho_{i+1,j}^a, \rho_{i,j+1}^a), \quad (359a)$$

where

$$\rho_{i,j}^a = \max (\rho_{i,j}^{TD}, \rho_{i,j}^n),$$

and

$$\rho_{i,j}^{\min} = \min (\rho_{i-1,j}^b, \rho_{i,j-1}^b, \rho_{i,j}^b, \rho_{i+1,j}^b, \rho_{j+1}^b), \quad (359b)$$

where

$$\rho_{i,j}^b = \min (\rho_{i,j}^{TD}, \rho_{i,j}^n).$$

#### ANTIDIFFUSION AND HALF-STEP UPDATING

The corrected antidiffusion fluxes are added

$$\psi_{i,j}^{n+1} \rho_{i,j}^{n+1} = \psi_{i,j}^{n+1} \rho_{i,j}^{TD} - (F_{i+\frac{1}{2},j}^C - F_{i-\frac{1}{2},j}^C) - (F_{i,j+\frac{1}{2}}^C - F_{i,j-\frac{1}{2}}^C) \quad (360)$$

thus giving the new density  $\rho_{i,j}^{n+1}$ .

Finally, it remains to specify  $u_{i+\frac{1}{2},j}^{n+\frac{1}{2}}$  and  $v_{i,j+\frac{1}{2}}^{n+\frac{1}{2}}$  in equations (340) and the source terms denoted by "source  $_{i,j}^{n+\frac{1}{2}}$ ." First, the velocities at the interfaces are obtained from

$$u_{i+\frac{1}{2},j}^{n+\frac{1}{2}} = \frac{u_{i,j}^{n+\frac{1}{2}} + u_{i+1,j}^{n+\frac{1}{2}}}{2} \quad (361a)$$

for  $i = 1, \dots, N_x - 1$  and  $j = 1, \dots, N_y$  while

$$u_{\frac{1}{2},j}^{n+\frac{1}{2}} = \frac{u_{i,j}^{n+\frac{1}{2}} + u_L}{2}$$

$$u_{N_x+\frac{1}{2},j}^{n+\frac{1}{2}} = \frac{u_{N_x,j}^{n+\frac{1}{2}} + u_R}{2}$$

and



$$v_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{v_{i,j}^{n+\frac{1}{2}} + v_{i,j+1}^{n+\frac{1}{2}}}{2} \quad (361b)$$

for  $i = 1, \dots, N_x$  and  $j = 1, \dots, N_y - 1$  while

$$v_{i,\frac{1}{2}}^{n+\frac{1}{2}} = \frac{v_{i,1}^{n+\frac{1}{2}} + v_B}{2}$$

$$v_{i,N_y+\frac{1}{2}}^{n+\frac{1}{2}} = \frac{v_{i,N_y}^{n+\frac{1}{2}} + v_T}{2}$$

As for the source terms they were defined earlier, Eqs. (321) through (329).

Next, to get  $u_{i,j}^{n+\frac{1}{2}}$ ,  $v_{i,j}^{n+\frac{1}{2}}$ , and source  $_{i,j}^{n+\frac{1}{2}}$ , we advance our system of conservation equations  $\frac{1}{2}$  time step using  $u_{i,j}^n$ ,  $v_{i,j}^n$ , source  $_{i,j}^n$ , then

$$u_{i,j}^{n+\frac{1}{2}} \Big|_{t \rightarrow t^n + \delta t} = u_{i,j}^{n+1} \Big|_{t \rightarrow t^n + \frac{\delta t}{2}}$$

$$v_{i,j}^{n+\frac{1}{2}} \Big|_{t \rightarrow t^n + \delta t} = v_{i,j}^{n+1} \Big|_{t \rightarrow t^n + \frac{\delta t}{2}}$$

$$\text{source}_{i,j}^{n+\frac{1}{2}} \Big|_{t \rightarrow t^n + \delta t} = \text{source}_{i,j}^{n+1} \Big|_{t \rightarrow t^n + \frac{\delta t}{2}}.$$

# XVII. TWO-DIMENSIONAL TIME SPLITTING VERSUS FULL TWO-DIMENSIONAL ALGORITHMS

Going back to Eq. (202),

$$A(\beta_x, \beta_y) = e^{-i(\epsilon_x \beta_x + \epsilon_y \beta_y)} = e^{-i\epsilon_x \beta_x} e^{-i\epsilon_y \beta_y} = A(\beta_x) A(\beta_y) \quad (362)$$

If  $\rho_{i,j}^n = e^{i\vec{k} \cdot \vec{x}}$ , where  $\vec{x} = (i\delta x, j\delta y)$ , the analytic solution of  $\frac{\partial \rho}{\partial t} + \vec{u} \cdot \nabla \rho = 0$ , according to Eq. (362), yields

$$\rho_{i,j}^{n+1} = A(\beta_y) A(\beta_x) \rho_{i,j}^n \quad (363)$$

where  $\vec{u} = (u, v)$  is constant and the two operators  $A(\beta_x)$  and  $A(\beta_y)$  are commutable. Noticing that

$$\rho_{i,j}^x = A(\beta_x) \rho_{i,j}^n \quad (364a)$$

is the analytic solution of  $\frac{\partial \rho}{\partial t} + u \frac{\partial \rho}{\partial x} = 0$ , whereas

$$\rho_{i,j}^{n+1} = A(\beta_y) \rho_{i,j}^x \quad (364b)$$

is the analytic solution of  $\frac{\partial \rho}{\partial t} + v \frac{\partial \rho}{\partial y} = 0$  for an initial density  $\rho_{i,j}^x$ , equation (363) invokes time splitting as an exact solution for the linear PDE. If we derive a numerical scheme by expanding  $A(\beta_x, \beta_y)$  in terms of  $\sin \beta_x$ ,  $\cos \beta_x$ ,  $\sin \beta_y$  and  $\cos \beta_y$  such that both  $A(\beta_x, \beta_y)$  and its expansion agree up to a prescribed order of  $\beta_x$  and  $\beta_y$ , we obviously end with a time splitting scheme, in which each of the x and y operators agrees with  $A(\beta_x)$  and  $A(\beta_y)$  up to a prescribed order of  $\beta_x$  and  $\beta_y$ , respectively.

Alternatively, if a 1-D scheme is n - order in phase error and m - order in diffusion error, namely

$$|A| = 1 + O(\beta^m) \quad (365)$$

and

$$\theta = \theta_{\text{exact}} + O(\beta^{n+1}) \quad (365b)$$

where  $|A|$  and  $\theta$  are the amplitude and angle of the scheme transfer function  $A$ , i.e.,  $A = |A| e^{i\theta}$ , using a time-splitted version of the one-dimensional scheme to solve a two-dimensional, x-y problem, gives  $|A| e^{i\theta} = A \equiv A_x A_y$   
 $= (|A_x| e^{i\theta_x}) (|A_y| e^{i\theta_y})$ . Thus,

$$|A| = |A_x| \cdot |A_y| = (1 + O(\beta_x^m)) (1 + O(\beta_y^m)) = 1 + O(\beta_x^m) + O(\beta_y^m) \quad (366a)$$

and

$$\begin{aligned} \theta &= \theta_x + \theta_y = [\theta_x^{\text{exact}} + O(\beta_x^{n+1})] + [\theta_y^{\text{exact}} + O(\beta_y^{n+1})] \\ &= \theta_{\text{exact}} + O(\beta_x^{n+1}) + O(\beta_y^{n+1}) \end{aligned} \quad (366b)$$

showing the two-dimensional scheme to be of the same order as the one-dimensional one. Moreover, the errors in both  $|A|$  and  $\theta$  are free from mixed frequencies, such as  $O(\beta_x^{n_1} \beta_y^{n_2})$  where  $n_1 + n_2 = m$  or  $n + 1$ .

Although time-splitting appears to be the perfect solution, physically unacceptable results are produced when dealing with incompressible or nearly incompressible flow fields, or when a differential identity, such as divergence free property or irrotationality, is to be strictly enforced. Moreover, because the antidiffusion fluxes are corrected in each direction independently of the other, unnecessary "clipping" occurs. Namely, the flux corrector may cancel a flux that would produce a ripple in one direction, which actually is safe in two-dimensions due to the growth or decay of the adjacent cells in the other direction.

Going back to the problems arising in incompressible flows, let's consider a case where  $\vec{U} = \vec{U}(x,y)$ , independent of time, satisfying  $\nabla \cdot \vec{U} = 0$ . For simplicity assume  $u = u_0 + Cx$  and  $v = v_0 - Cy$ . Figure 41 illustrates the velocities at the interfaces of a cell, when  $\delta x = \delta y = 1$ ,  $C = 0.1$ .

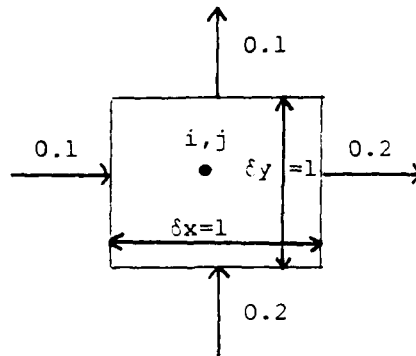


Fig. 41

Using a simple-transport scheme with time splitting

$$\psi_{i,j} \rho_{i,j}^x = \psi_{i,j} \rho_{i,j}^0 - (u_{i+\frac{1}{2},j} \rho_{i+\frac{1}{2},j}^0 - u_{i-\frac{1}{2},j} \rho_{i-\frac{1}{2},j}^0) \delta y \delta t \quad (367a)$$

$$\psi_{i,j} \rho_{i,j}^1 = \psi_{i,j} \rho_{i,j}^x - (v_{i,j+\frac{1}{2}} \rho_{i,j+\frac{1}{2}}^x - v_{i,j-\frac{1}{2}} \rho_{i,j-\frac{1}{2}}^x) \delta x \delta t \quad (367b)$$

where 0,1 stands for  $t = 0, \delta t$ , respectively. Assuming a uniform initial density  $\rho^0 = 1$ , and  $\delta t = 1$ , Eq. (367a) gives  $(1) \cdot (\rho_{i,j}^x) = (1) \cdot (1) - ((0.2) \cdot (1) - (0.1) \cdot (1)) \cdot (1) \cdot (1)$  yielding  $\rho_{i,j}^x = 0.9$ . Since  $u = u(x)$ ,  $v = v(y)$ ,  $\rho_{i,j}^x = 0.9$  for all  $j$ 's and since  $u, v$  are linear, it is also true for all  $i$ 's. Then, from Eq. (367b), we obtain  $(1) \cdot (\rho_{i,j}^1) = (1) \cdot (0.9) - ((0.1) \cdot (0.9) - (0.2) \cdot (0.9)) \cdot (1) \cdot (1)$  yielding  $\rho_{i,j}^1 = 0.99$ . After  $n$  time steps, it is obvious that  $\rho_{i,j}^n = (0.99)^n$  for all  $i$  and  $j$ . Generally,  $\rho_{i,j}^n = \rho_{i,j}^0 (1-C^2)^n$ . In other words, the density keeps on uniformly distributed but decreases with time continuously.

An equivalent fully two-dimensional scheme would be

$$\begin{aligned} \psi_{i,j} \rho_{i,j}^1 = & \psi_{i,j} \rho_{i,j}^0 - (u_{i+\frac{1}{2},j} \rho_{i+\frac{1}{2},j}^0 - u_{i-\frac{1}{2},j} \rho_{i-\frac{1}{2},j}^0) \delta y \delta t \\ & - (v_{i,j+\frac{1}{2}} \rho_{i,j+\frac{1}{2}}^0 - v_{i,j-\frac{1}{2}} \rho_{i,j-\frac{1}{2}}^0) \delta x \delta t \end{aligned} \quad (368)$$

which gives  $\rho_{i,j}^1 = 1$ , i.e. conserves the mass.

The discrepancy obviously lies in the assumption of  $\vec{U} = \text{const}$  while  $\rho$  is varying when deriving Eq. (362). In terms of transfer functions, the scheme of Eqs. (367) is written as  $A = (1 - \varepsilon_x t_x)(1 - \varepsilon_y t_y)$  whereas that of Eq. (368) takes the form  $A = 1 - \varepsilon_x t_x - \varepsilon_y t_y$ .

The difference is obviously in the term " $\varepsilon_x \varepsilon_y t_x t_y$ " which as will be shown later is essential for high order diffusion. In the next section, we try to cast a time-splitted scheme into a fully two-dimensional form. A detailed explanation of the problems involved is given.

#### FULLY TWO-DIMENSIONAL VERSIONS OF TIME-SPLITTED SCHEMES

Going back to the fourth order phase and diffusion scheme

$$A = (1 - \varepsilon t)(1 - \mu d) + \nu d \quad (370)$$

where  $\nu = \frac{1}{6} + \frac{\varepsilon^2}{3}$  and  $\mu = \frac{1-\varepsilon^2}{6}$ . The two-dimensional, splitted version of Eq. (370)

$$A = [(1 - \varepsilon_x t_x)(1 - \mu_x d_x) + \nu_x d_x] \cdot [(1 - \varepsilon_y t_y)(1 - \mu_y d_y) + \nu_y d_y] \quad (371a)$$

or

$$\begin{aligned}
A = & (1 - \epsilon_x t_x + v_x d_x)(1 - \epsilon_y t_y + v_y d_y) - u_x d_x(1 - \epsilon_x t_x)(1 - \epsilon_y t_y + v_y d_y) \\
& - v_y d_y(1 - \epsilon_y t_y)(1 - \epsilon_x t_x + v_x d_x) - u_x v_y d_x d_y(1 - \epsilon_x t_x)(1 - \epsilon_y t_y)
\end{aligned}
\tag{371b}$$

can be written as

$$\begin{aligned}
A^{TD} = & 1 - \epsilon_x t_x \left(1 - \frac{\epsilon_y t_y}{2} + \frac{v_y d_y}{2}\right) - \epsilon_y t_y \left(1 - \frac{\epsilon_x t_x}{2} + \frac{v_x d_x}{2}\right) \\
& + v_x d_x \left(1 - \frac{\epsilon_y t_y}{2} + \frac{v_y d_y}{2}\right) + v_y d_y \left(1 - \frac{\epsilon_x t_x}{2} + \frac{v_x d_x}{2}\right)
\end{aligned}
\tag{372a}$$

which is  $\geq 0$  for  $|\epsilon_x|, |\epsilon_y| \leq \frac{1}{2}$ , therefore ensuring positivity of  $\rho^{TD}$  if  $\rho^n \geq 0$ . Then,

$$\begin{aligned}
A = A^{TD} - u_x d_x^* (1 - \epsilon_x t_x) [1 - \epsilon_y t_y + v_y d_y - \frac{1}{2} u_y d_y (1 - \epsilon_y t_y)] \\
- v_y d_y^* (1 - \epsilon_y t_y) [1 - \epsilon_x t_x + v_x d_x - \frac{1}{2} u_x d_x (1 - \epsilon_x t_x)]
\end{aligned}
\tag{372b}$$

where the asterisks denote the operators which fluxes are to be corrected. This will allow us to correct the x and y antidiffusion fluxes simultaneously, thus avoiding unnecessary clipping. But that does not solve the problems associated with divergence free flow fields, for example, because of the term " $\epsilon_x \epsilon_y t_x t_y$ ." Moreover, we notice that the form of Eq. (372) is in no way unique.

Although Eqs. (366) show in a clear simple way that  $A \equiv A_x A_y$  is fourth order in phase and diffusion, let us analyze it using Eqs. (246) to (248), Eqs. (260)-(262) with Eqs. (241)-(244). The purpose is to determine which terms are responsible for the fourth order diffusion, fourth order phase error, positivity, stability, and so on. We notice that  $A^{t_x t_x} = 0$ ,  $A^{t_y t_y} = 0$ , making Eqs. (241)-(244) valid.

Differentiating Eq. (371a), we get

$$A_{\bar{Y}}^t = -\epsilon_{\bar{X}}(1 - \mu_{\bar{X}}^d) A_{\bar{X}}^t \quad (374)$$

$$A_{\bar{Y}}^d = [(v_{\bar{X}} - \mu_{\bar{X}}) + \epsilon_{\bar{X}} \mu_{\bar{X}}^t] A_{\bar{X}}^t \quad (375)$$

$$A_{\bar{Y}\bar{Y}}^{t d} = \epsilon_{\bar{X}} \mu_{\bar{X}}^t A_{\bar{X}}^t \quad (376)$$

$$A_{\bar{Y}\bar{X}}^{t d} = -\epsilon_{\bar{X}}(1 - \mu_{\bar{X}}^d) [(v_{\bar{Y}} - \mu_{\bar{Y}}) + \epsilon_{\bar{Y}} \mu_{\bar{Y}}^t] \quad (377)$$

$$A_{\bar{X}\bar{Y}}^{t t} = \epsilon_{\bar{X}} \epsilon_{\bar{Y}} (1 - \mu_{\bar{X}}^d) (1 - \mu_{\bar{Y}}^d) \quad (378a)$$

$$A_{\bar{X}\bar{Y}}^{d d} = [(v_{\bar{X}} - \mu_{\bar{X}}) + \epsilon_{\bar{X}} \mu_{\bar{X}}^t] [(v_{\bar{Y}} - \mu_{\bar{Y}}) + \epsilon_{\bar{Y}} \mu_{\bar{Y}}^t] \quad (378b)$$

At  $\beta_{\bar{X}} = \beta_{\bar{Y}} = 0$ ,  $t_{\bar{X}} = t_{\bar{Y}} = 0$ , and  $d_{\bar{X}} = d_{\bar{Y}} = 0$ , thus  $A_{\bar{X}} = A_{\bar{Y}} = 1$ , yielding

$$A_{\bar{O}}^t = -\epsilon_{\bar{X}} \quad (379)$$

$$A_{\bar{O}}^d = v_{\bar{X}} - \mu_{\bar{X}} \quad (380)$$

$$A_{\bar{O}}^{t d} = \epsilon_{\bar{X}} \mu_{\bar{X}}^t \quad (381)$$

$$A_{\bar{O}}^{t d} = -\epsilon_{\bar{X}} (v_{\bar{Y}} - \mu_{\bar{Y}}) \quad (382)$$

$$A_{\bar{O}}^{t t} = \epsilon_{\bar{X}} \epsilon_{\bar{Y}} \quad (383a)$$

$$A_{\bar{O}}^{d d} = (v_{\bar{X}} - \mu_{\bar{X}}) (v_{\bar{Y}} - \mu_{\bar{Y}}) \quad (383b)$$

Substituting into Eqs. (246) and (248), we get

$$(\log A)_{\frac{0}{Y}}^{\frac{X}{Y}} = -i\epsilon_{\frac{X}{Y}} \quad (384)$$

$$\begin{aligned} (\log A)_{\frac{0}{YY}}^{\frac{XXX}{YYY}} &= i\epsilon_{\frac{X}{Y}} [1 - 6(v_{\frac{X}{Y}} - \mu_{\frac{X}{Y}})] - i[6\epsilon_{\frac{X}{Y}} u_{\frac{X}{Y}} - 2\epsilon_{\frac{X}{Y}}^3] \\ &= 6i\epsilon_{\frac{X}{Y}} \left( \frac{1}{6} + \frac{\epsilon_{\frac{X}{Y}}^2}{3} - v_{\frac{X}{Y}} \right) \end{aligned} \quad (385)$$

showing  $A_{\frac{X}{Y}} A_{\frac{Y}{Y}}$  to be fourth order in phase error, but more importantly, that the cross terms of Eqs. (382) and (393a), which do not appear in one-dimension, are essential to the fourth order phase. More specifically, these cross terms reduce the dependence of phase error on  $v$  and  $u$  to dependence on  $v$  only, leaving  $\mu$  free to be adjusted for a high order diffusion.

$A_{\frac{0}{X}}^{\frac{d}{d} \frac{d}{d} \frac{d}{d} \frac{d}{d}}$  in Eq. (383b) is not used in either (384) or (385) and therefore can take any value without affecting the phase error.

Now we can construct the simplest fourth order phase error scheme. Such a scheme has to satisfy Eqs. (379) to (382) plus Eq. (383a) giving,

$$\begin{aligned} A &= (1 - \epsilon_{\frac{X}{X}} t_x)(1 - \epsilon_{\frac{Y}{Y}} t_y) + (v_{\frac{X}{X}} - \mu_{\frac{X}{X}}) d_x + (v_{\frac{Y}{Y}} - \mu_{\frac{Y}{Y}}) d_y + \epsilon_{\frac{X}{X}} t_x u_{\frac{X}{X}} d_x \\ &\quad + \epsilon_{\frac{Y}{Y}} t_y u_{\frac{Y}{Y}} d_y - \epsilon_{\frac{X}{X}} t_x (v_{\frac{Y}{Y}} - \mu_{\frac{Y}{Y}}) d_y - \epsilon_{\frac{Y}{Y}} t_y (v_{\frac{X}{X}} - \mu_{\frac{X}{X}}) d_x \end{aligned} \quad (386)$$

where the integration constant was selected as unity to satisfy consistency, i.e.,  $A(\beta_{\frac{X}{X}}, \beta_{\frac{Y}{Y}} = 0) = 1$ . Eq. (386) can be written as

$$\begin{aligned} A &= (1 - \epsilon_{\frac{X}{X}} t_x)(1 - \epsilon_{\frac{Y}{Y}} t_y) + v_{\frac{X}{X}} d_x (1 - \epsilon_{\frac{Y}{Y}} t_y) + v_{\frac{Y}{Y}} d_y (1 - \epsilon_{\frac{X}{X}} t_x) \\ &\quad - \mu_{\frac{X}{X}} d_x (1 - \epsilon_{\frac{X}{X}} t_x - \epsilon_{\frac{Y}{Y}} t_y) - \mu_{\frac{Y}{Y}} d_y (1 - \epsilon_{\frac{X}{X}} t_x - \epsilon_{\frac{Y}{Y}} t_y) \end{aligned} \quad (387)$$



Since  $A_{00}^{dd}$  does not affect the phase error order, we can assign a value for it that would ensure positivity. We add to the terms of Eq. (387)

" $v_{xy} d_x d_y$ ," yielding

$$A = (1 - \epsilon_x t_x + v_{xx} d_x)(1 - \epsilon_y t_y + v_{yy} d_y) - \mu_{xx} d_x (1 - \epsilon_x t_x - \epsilon_y t_y) - \mu_{yy} d_y (1 - \epsilon_x t_x - \epsilon_y t_y) \quad (388)$$

Now, substituting Eqs. (379) to (383) into Eqs. (242) and (243), we get

$$A_{00}^{xy} = -i \epsilon_{xy} \quad (389)$$

$$A_{00}^{xx} = -2(v_{xx} - \mu_{xx}) \quad (390a)$$

$$A_{00}^{xy} = -\epsilon_x \epsilon_y \quad (390b)$$

which when substituted into Eqs. (261), yield

$$(|A|_{00}^{xx})^2 = 2[-2(v_{xx} - \mu_{xx}) + \epsilon_x^2] = 0 \quad (391a)$$

$$(|A|_{00}^{xy})^2 = 2[-\epsilon_x \epsilon_y + \epsilon_x^2] = 0 \quad (391b)$$

showing  $A_{xy}$  to be fourth order in diffusion error.

Notice that  $A_{00}^{tx ty} = \epsilon_x \epsilon_y$ , is essential for fourth order diffusion (already satisfied by the scheme of Eq. (388)).

The simplest fourth order (phase and diffusion error) positive scheme is therefore that of Eq. (388). It is, however, unstable. For instance,

$$A_R = 1 + (v_x - \mu_x)d_x + (v_y - \mu_y)d_y + v_x v_y d_x d_y + \varepsilon_x \varepsilon_y t_x t_y \quad (392a)$$

while

$$A_I = -\varepsilon_x t_x [1 - \mu_x d_x + (v_y - \mu_y)d_y] - \varepsilon_y t_y [1 - \mu_y d_y + (v_x - \mu_x)d_x] \quad (392b)$$

At  $\varepsilon_x = \varepsilon_y = \frac{1}{2}$  and  $\beta_x = \beta_y = \pi/2$ ,  $d_x = d_y = -2$ , and  $t_x = t_y = i$ , yielding

$$A_R = 1 - \frac{1}{4} - \frac{1}{4} + \frac{1}{4} - \frac{1}{4} = \frac{1}{2} \quad (393a)$$

$$A_I = -\frac{1}{2}[1 + \frac{1}{4} - \frac{1}{4}] - \frac{1}{2}[1 + \frac{1}{4} - \frac{1}{4}] = -1 \quad (393b)$$

Since we know that A of Eq. (372) is stable, let's try to approach it in steps. First, we try

$$\begin{aligned} A = & (1 - \varepsilon_x t_x + v_x d_x)(1 - \varepsilon_y t_y + v_y d_y) - \mu_x d_x (1 - \varepsilon_x t_x)(1 - \varepsilon_y t_y) \\ & - \mu_y d_y (1 - \varepsilon_y t_y)(1 - \varepsilon_x t_x) \end{aligned} \quad (394)$$

thus adding " $-(\mu_x d_x + \mu_y d_y)(\varepsilon_x \varepsilon_y t_x t_y)$ " to the real part, becoming then

$$A_R = 1/2 - 1/8 = 3/8 \quad (395)$$

still unstable. Next, we try

$$\begin{aligned} A = & (1 - \varepsilon_x t_x + v_x d_x)(1 - \varepsilon_y t_y + v_y d_y) - \mu_x d_x (1 - \varepsilon_x t_x)(1 - \varepsilon_y t_y + v_y d_y) \\ & - \mu_y d_y (1 - \varepsilon_y t_y)(1 - \varepsilon_x t_x + v_x d_x) \end{aligned} \quad (396)$$

This will add " $-(\mu_x v_y + \mu_y v_x)d_x d_y$ " to the real part and " $(\varepsilon_x t_x \mu_x v_y + \varepsilon_y t_y \mu_y v_x)d_x d_y$ " to the imaginary one. We get then

$$A_R = \frac{3}{8} - \frac{1}{4} = \frac{1}{8} \quad (397a)$$

$$A_I = -1 + \frac{1}{8} = -\frac{7}{8} \quad (397b)$$

whence  $|A|^2 = (\frac{7}{8})^2 + (\frac{1}{8})^2 = \frac{50}{64} < 1$ , showing Eq. (396) to be too stable at  $\beta_x = \beta_y = \frac{\pi}{2}$ . Moreover, it is not phoenical;  $A \neq 1$  at  $\epsilon_x = \epsilon_y = 0$ . These two effects can be avoided by picking

$$A = (1 - \epsilon_x t_x + v_x d_x)(1 - \epsilon_y t_y + v_y d_y) - \mu_x d_x (1 - \epsilon_x t_x)(1 - \epsilon_y t_y + \frac{1}{2} v_y d_y) - \mu_y d_y (1 - \epsilon_y t_y)(1 - \epsilon_x t_x + \frac{1}{2} v_x d_x) \quad (398)$$

yielding

$$A_R = \frac{3}{8} - \frac{1}{2} \times \frac{1}{4} = \frac{1}{4} \quad (399a)$$

$$A_I = -1 + \frac{1}{2} \times \frac{1}{8} = -\frac{15}{16} \quad (399b)$$

whence  $|A|^2 = (\frac{15}{16})^2 + (\frac{1}{4})^2 = \frac{241}{256} < 1$ , closer to 1, therefore promising a smaller net diffusion and phoenical since  $A = 1$  at  $\epsilon_x = \epsilon_y = 0$ .

Noticing that the added terms to Eq. (388) are triple operators

$(t_x t_y d_x, t_x t_y d_y, t_x d_x d_y, t_y d_y d_x)$  they have no effect on  $(\log A)_0'''$ .

Eq. (398) is still fourth order in phase error. Furthermore, upon expanding  $|A|^2$ , we get

$$|A|^2 = 1 + \frac{1}{12} \{ \epsilon_x^2 (1 - \epsilon_x^2) \beta_x^4 + [ \epsilon_x^2 (1 - \epsilon_y^2) + \epsilon_y^2 (1 - \epsilon_x^2) ] \beta_x^2 \beta_y^2 + \epsilon_y^2 (1 - \epsilon_y^2) \beta_y^4 \} + \dots \quad (400)$$

showing diffusion error to be of fourth order. The scheme is, however, slightly unstable near  $\beta_x = \beta_y = 0$ , since the fourth order coefficient is

positive. We notice also the presence of a term " $\beta_x^2 \beta_y^2$ " in Eq. (400) (also in the phase error expansion), which does not show in the expansion of Eq. (372) (according to Eq. (366), making the scheme of Eq. (398) slightly inferior to that of Eq. (372).

Upon comparing Eq. (398) to (372), it is obvious that Eq. (372) cannot be much simplified; at least without sacrificing stability or phoenicity. Whichever we use, the  $n^\circ$  of operations involved in evaluating  $\phi^{n+1}$  is much larger than that in the fully two-dimensional scheme of Eq. (226e). Moreover, the  $n^\circ$  of two-dimensional arrays required to store the intermediate values is enormous.

Since the only advantage of Eqs. (372), the fully two-dimensional version of the time-splitted scheme of Eq. (371b) is the reduced clipping associated with the flux limiter, we conclude that time splitting is the sensible answer. We abandon, therefore, trials to cast the time-splitted scheme in fully two-dimensional versions.

# XVIII. IMPROVING DIFFUSION ERROR OF THE FULLY TWO-DIMENSIONAL SCHEME

Now that we have classified the terms responsible for the fourth order phase, diffusion, etc., in the time-splitting scheme, let's go back to the fully two-dimensional scheme and study the terms preventing us from reaching a fourth order diffusion error. As explained earlier, the term " $\epsilon_x \epsilon_y t_x t_y$ " is essential to reduce the dependence of the phase error to one on  $v$  alone, thus leaving  $\mu$  free to be adjusted for a high order diffusion. A closer look reveals, however, that the above conclusion is an indirect one. The direct conclusion is that " $\epsilon_x \epsilon_y t_x t_y$ " is needed to cancel " $\epsilon_x \beta_x \epsilon_y \beta_y$ " resulting from squaring the imaginary part. Specifically, any scheme has to incorporate the combination  $(\epsilon_x t_x + \epsilon_y t_y)$  leading to  $i(\epsilon_x \sin \beta_x + \epsilon_y \sin \beta_y)$  which is approximated by  $i(\epsilon_x \beta_x + \epsilon_y \beta_y)$ . To cancel it, a term including  $\sin \beta_x \sin \beta_y$  is needed. Besides  $t_x t_y$ , the above term can also result from  $\cos(\beta_x \pm \beta_y)$ , i.e. diagonal diffusion  $(\rho_{i+1,j\pm 1}^n - 2\rho_{i,j}^n + \rho_{i-1,j\mp 1}^n)$ . Admitting diagonal terms is outside the scope of this article and is left out to an upcoming one. However, we emphasize that there is a stability problem caused by the imaginary part  $iA_I = -[\epsilon_x t_x (1 - \mu_x d_x) + \epsilon_y t_y (1 - \mu_y d_y)]$  which amplitude is already larger than unity for  $\epsilon_x = \epsilon_y = \frac{1}{2}$ ,  $\beta_x = \beta_y = \frac{\pi}{2}$  unless  $\mu_x = \mu_y = 0$  there, in which case we have a large residual diffusion. Adding just a diagonal diffusion can't help, since it only adds to the real part.

## REFERENCES

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2. Book, D. L., Boris, J. P., and Hain, K. H. (1975), "Flux-Corrected Transport II: Generalizations of the Method," J. Comp. Phys. 18, 248-283.
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4. Boris, J. P. and Book, D. L. (1976). "Solution of Continuity Equations by the Method of Flux-Corrected Transport," Chapter 11, Vol. 16 Methods of Computational Physics, Academic Press, New York.
5. Zalesak, S. T. (1979). "Fully Multidimensional Flux-Corrected Transport Algorithms for Fluids," J. Comp. Phys. 31, 335-362.

*FIGURES*

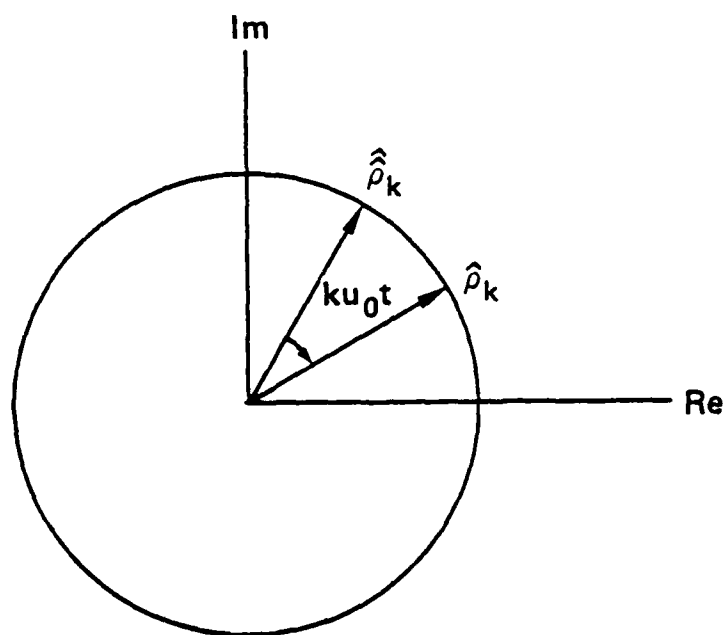


Fig. 1

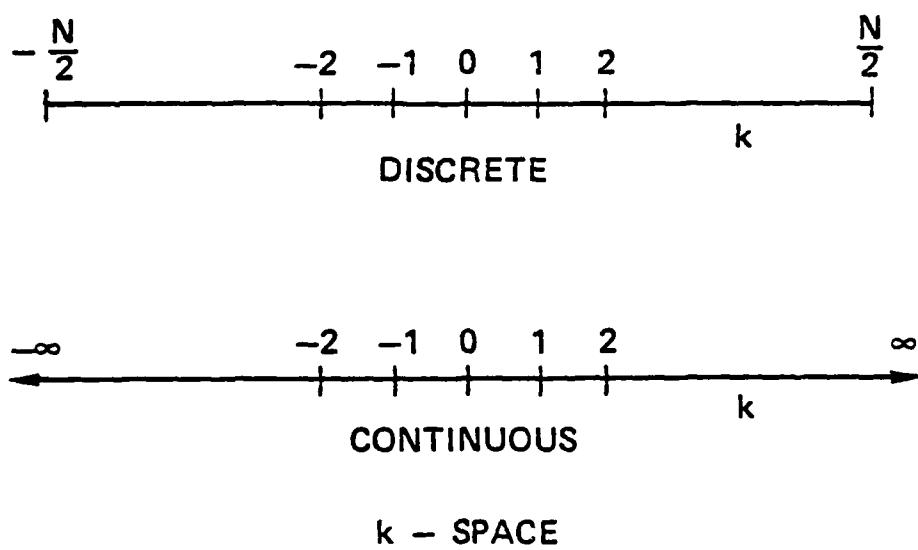


Fig. 2



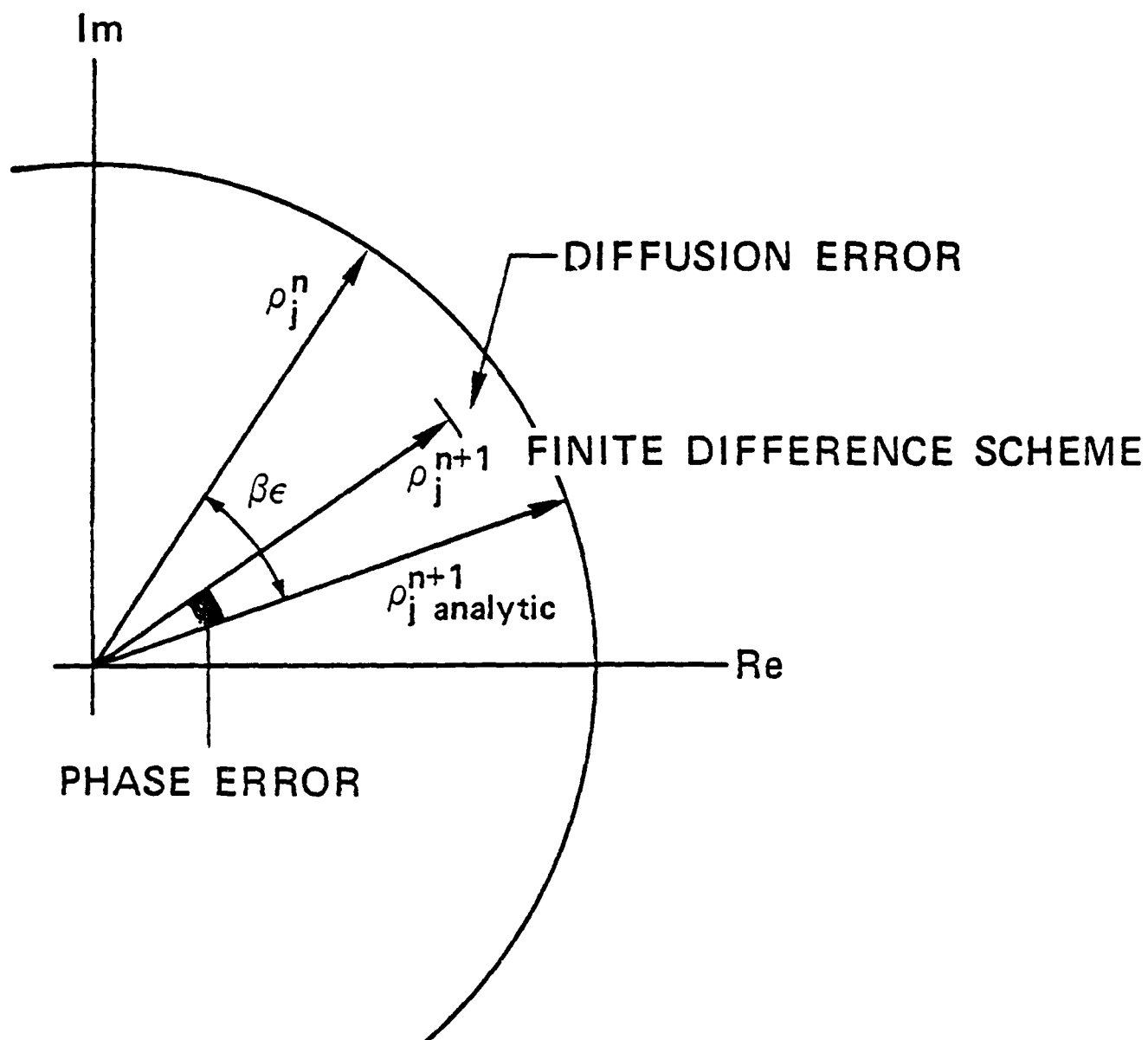


Fig. 3

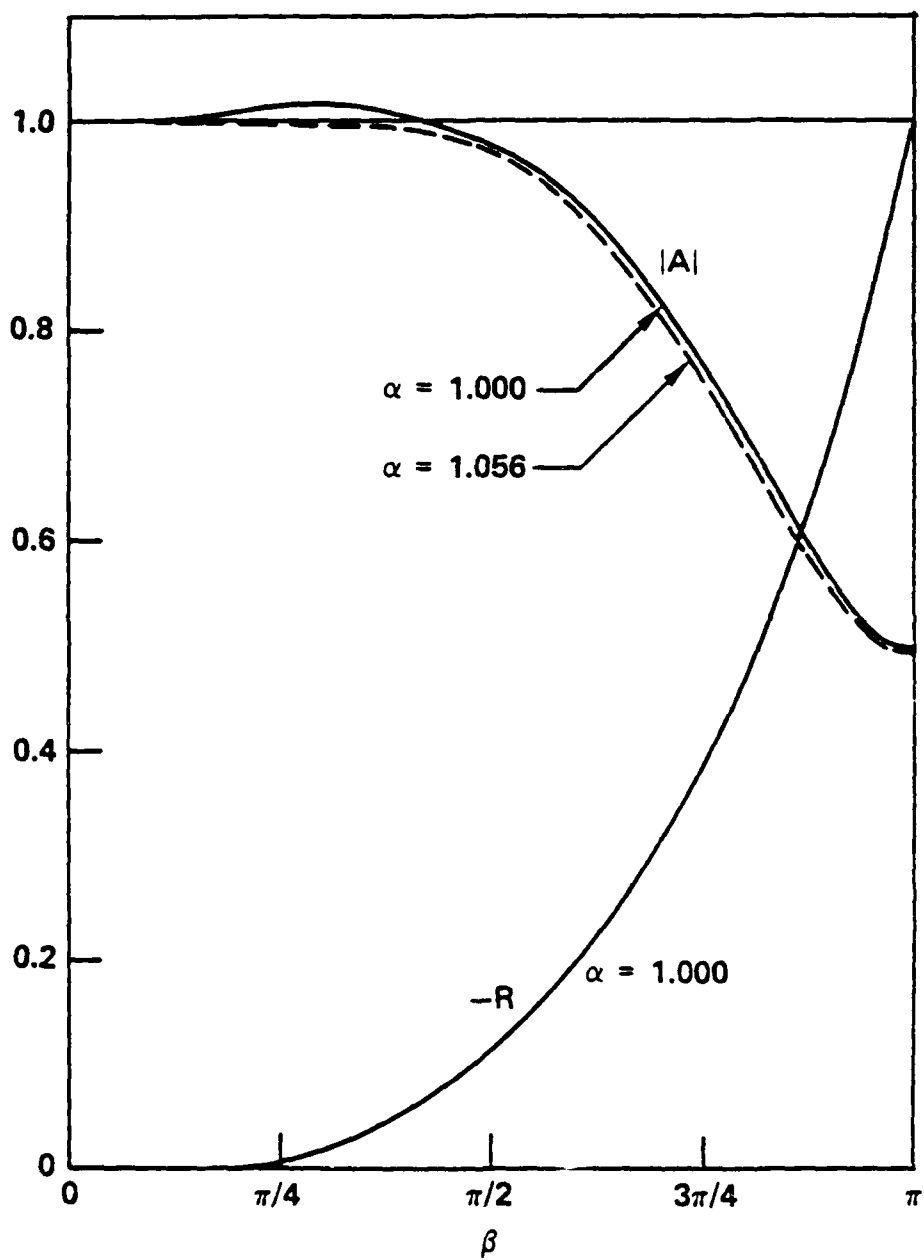
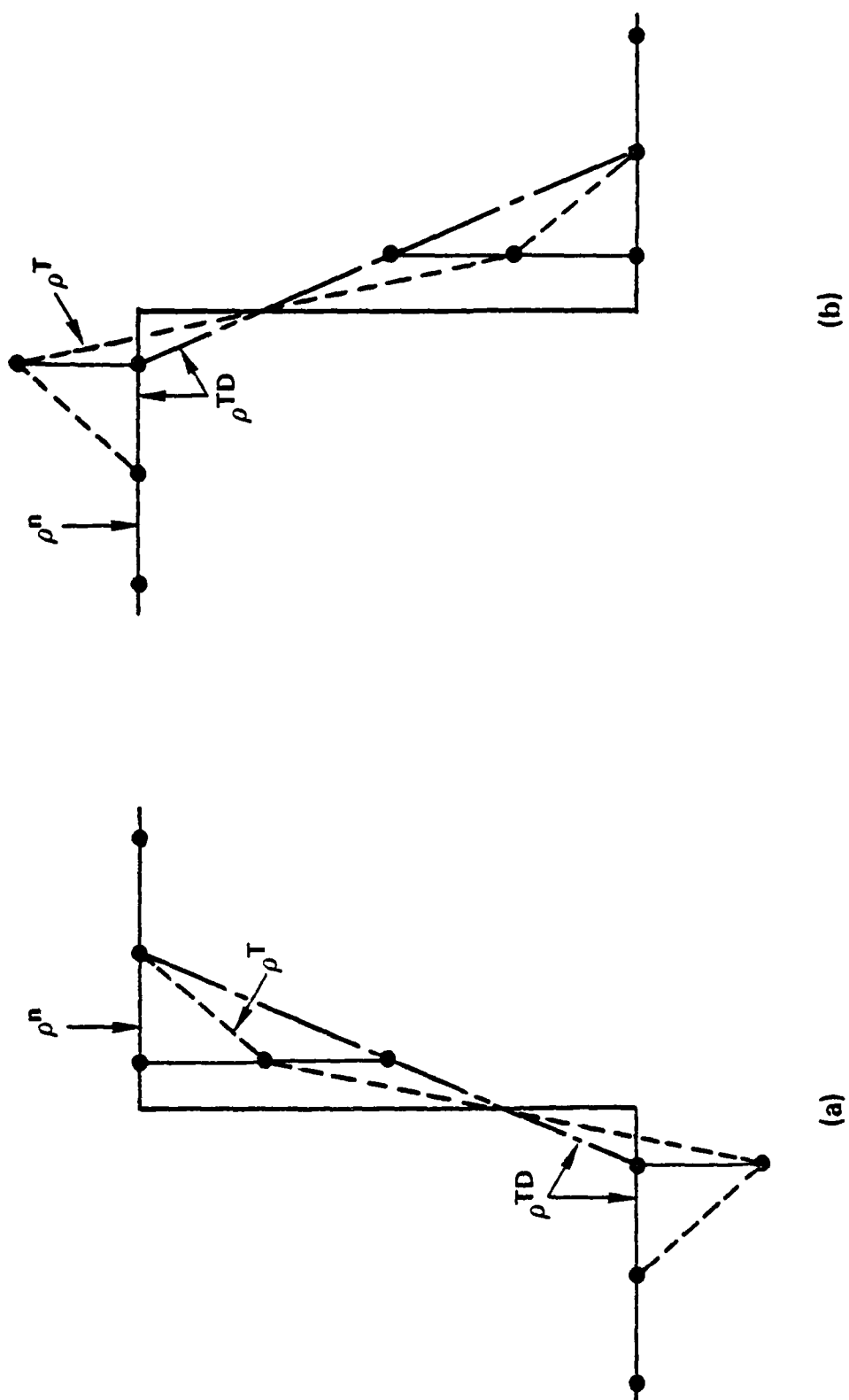


Fig. 4



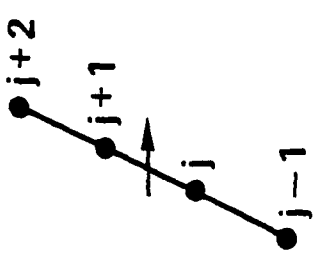
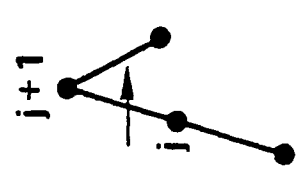
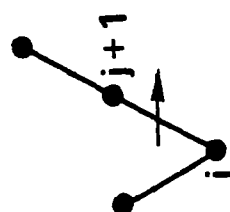
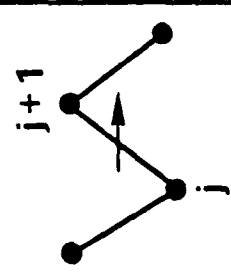
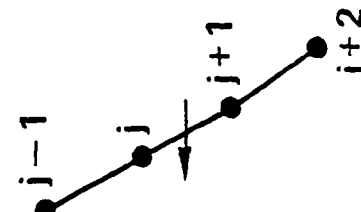
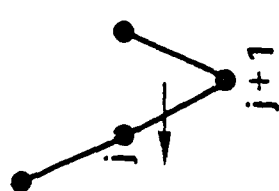
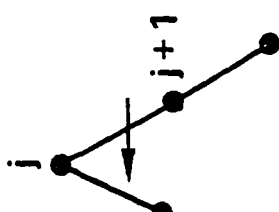
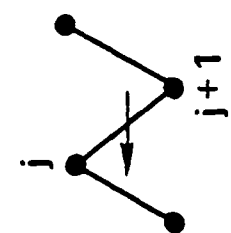
$f_{j+1}^{j+1} > 0$	 <p>(1)</p>	 <p>(2)</p>	 <p>(3)</p>	 <p>(4)</p>	LIMITED
$f_{j+1}^{j+1} < 0$	 <p>(5)</p>	 <p>(6)</p>	 <p>(7)</p>	 <p>(8)</p>	CANCELLED

Fig. 6

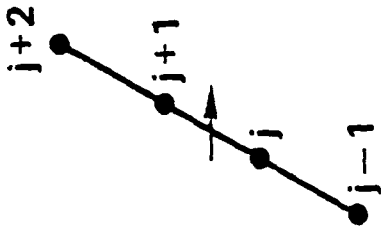
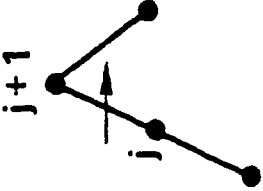
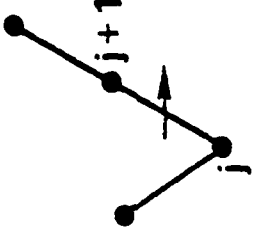
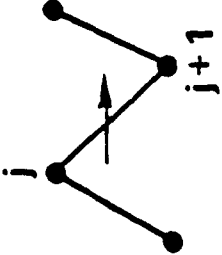
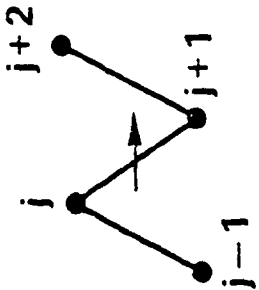
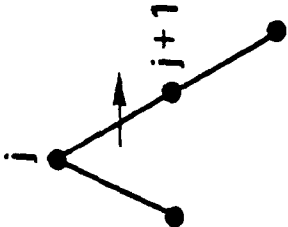
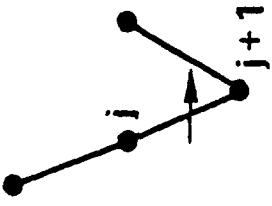
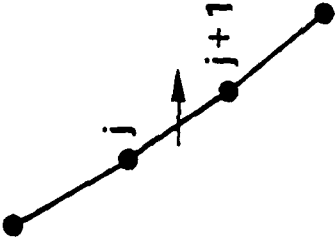
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$f_{j+\frac{1}{2}}$ OPPOSITE TO $\Delta_{j+\frac{1}{2}}$	 <p>(5)</p>	 <p>(6)</p>	 <p>(7)</p>	 <p>(8)</p>	<p>CANCELLED</p>

Fig. 7

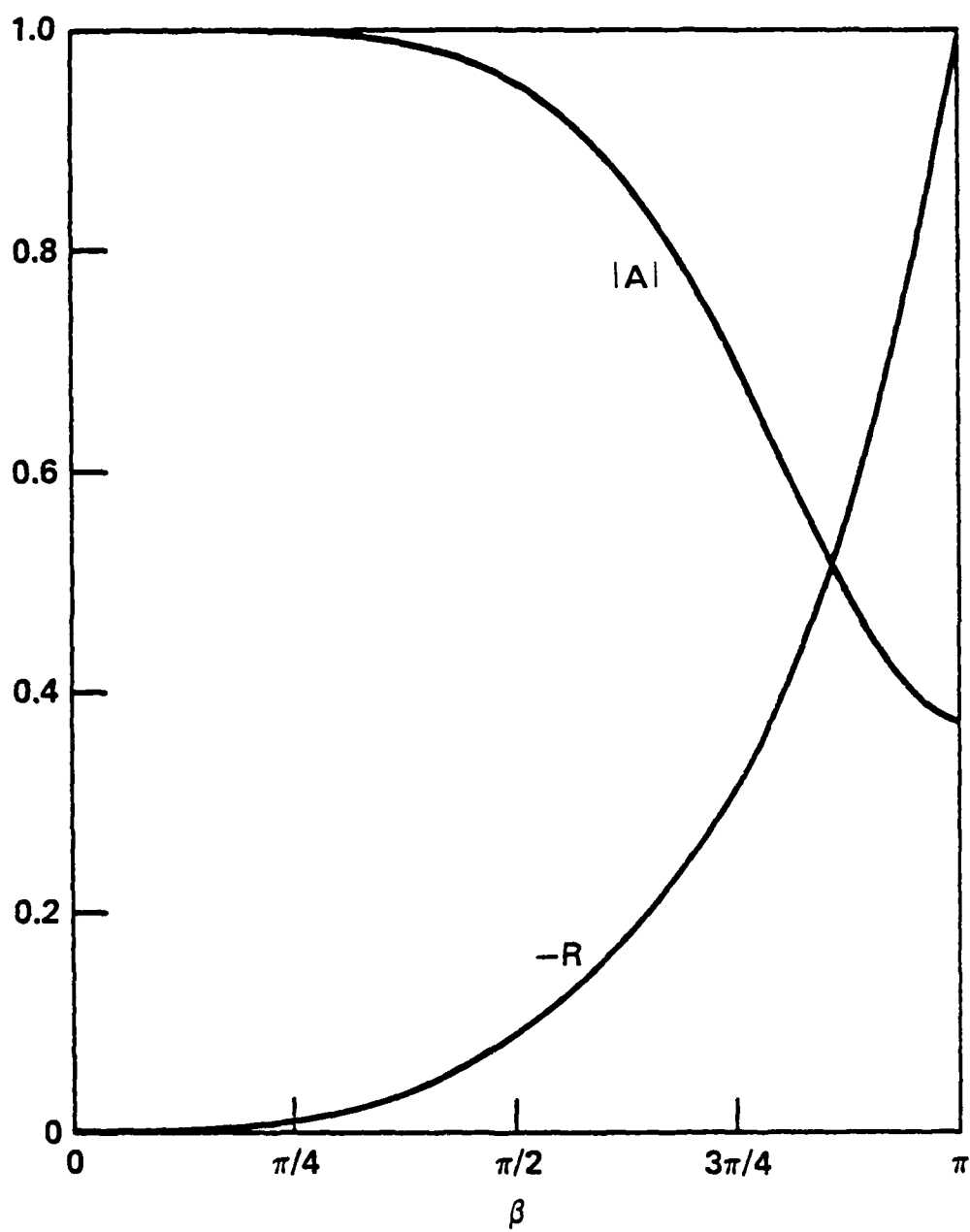


Fig. 3

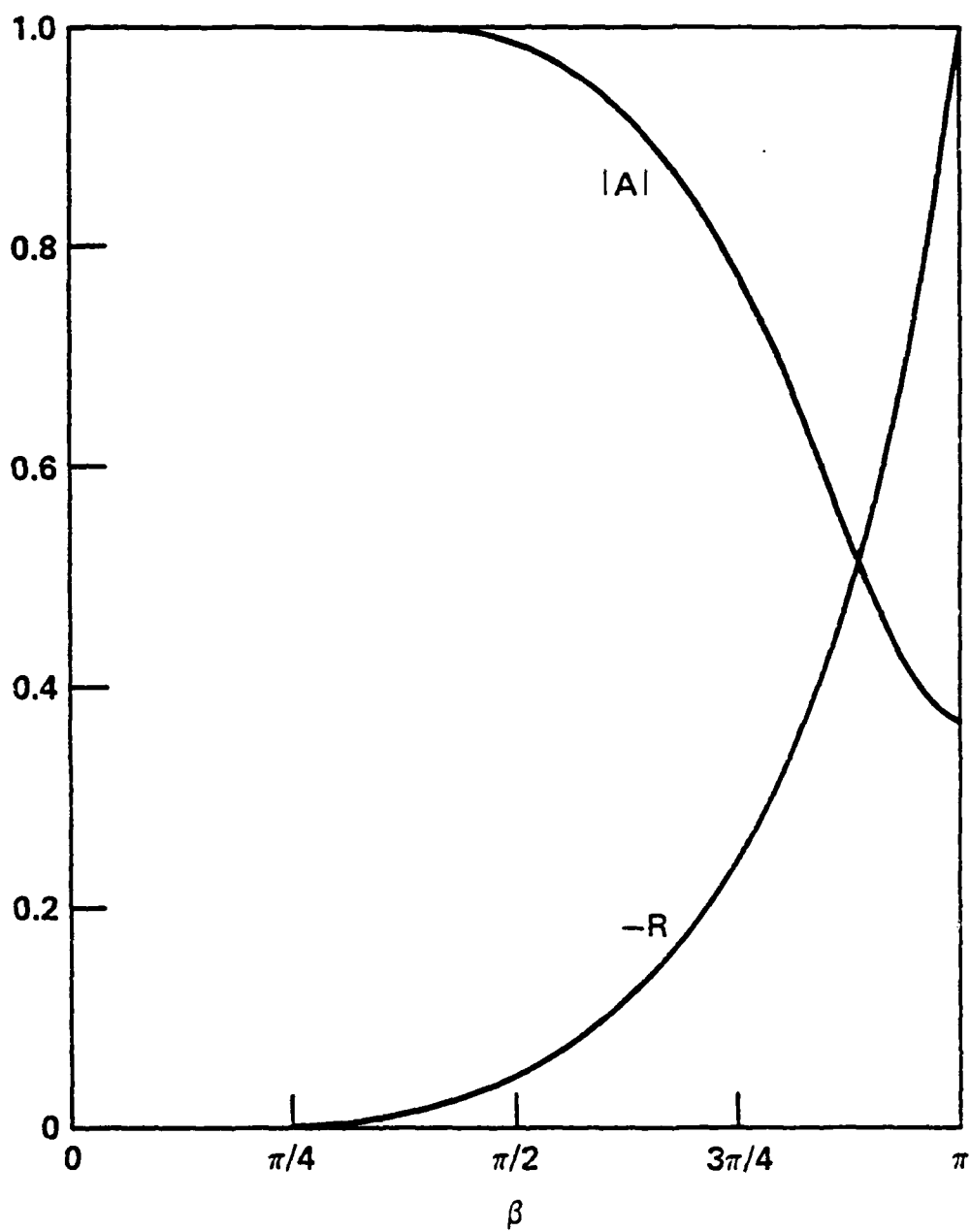


Fig. 2

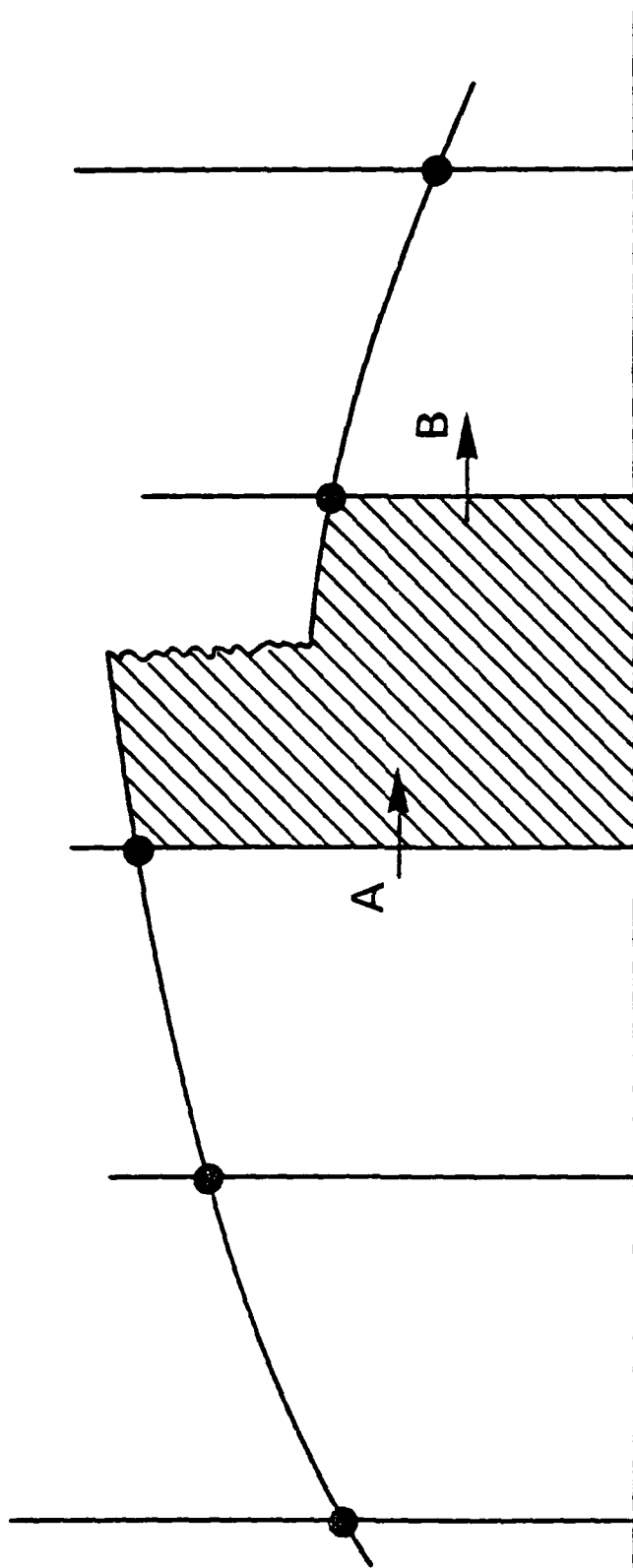


Fig. 10



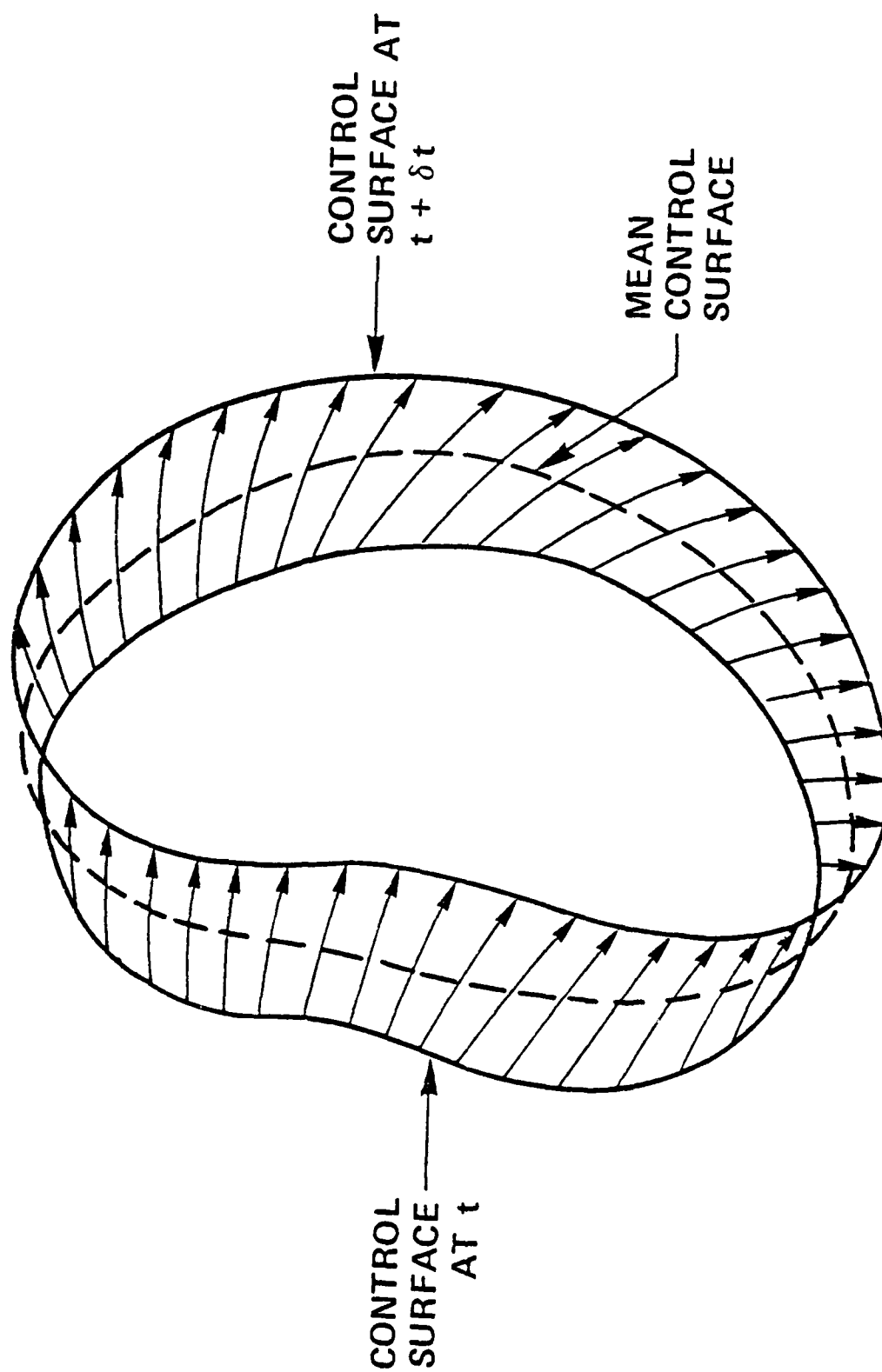


Fig. 11

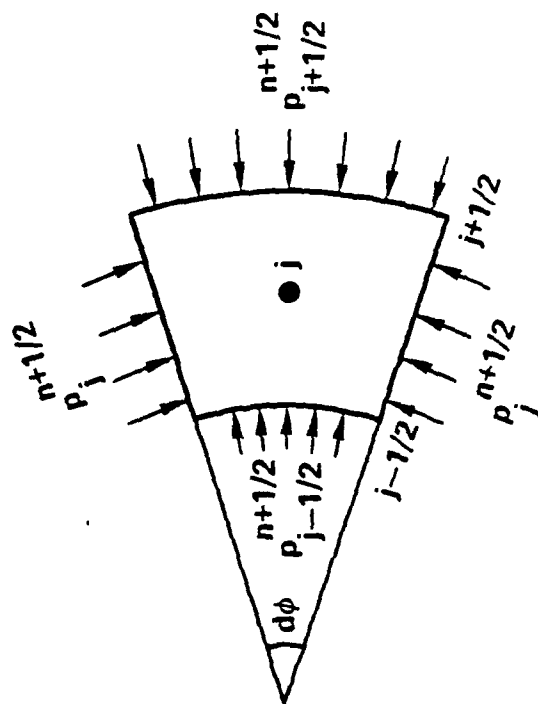


Fig. 13

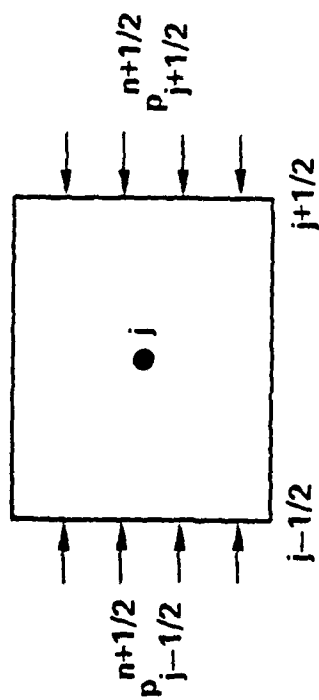


Fig. 12

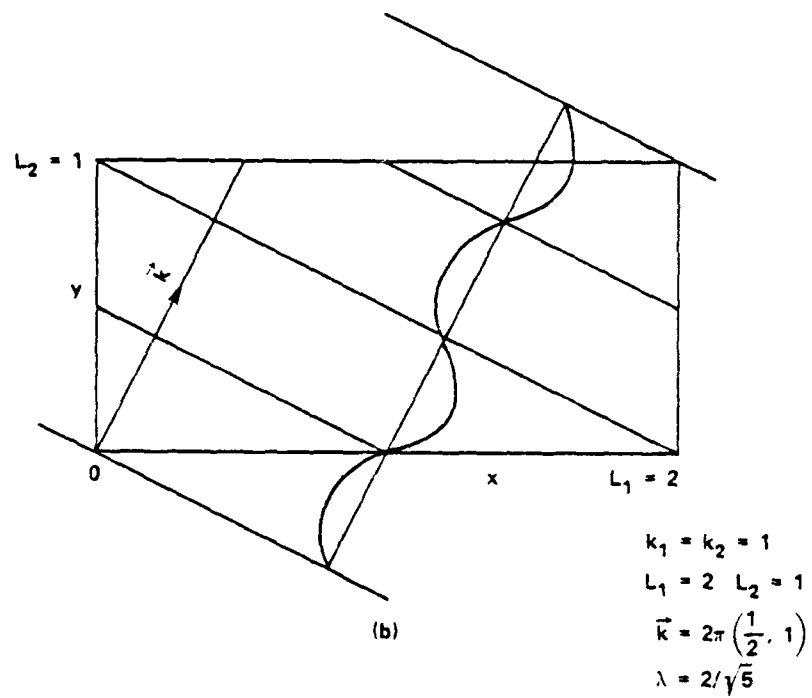
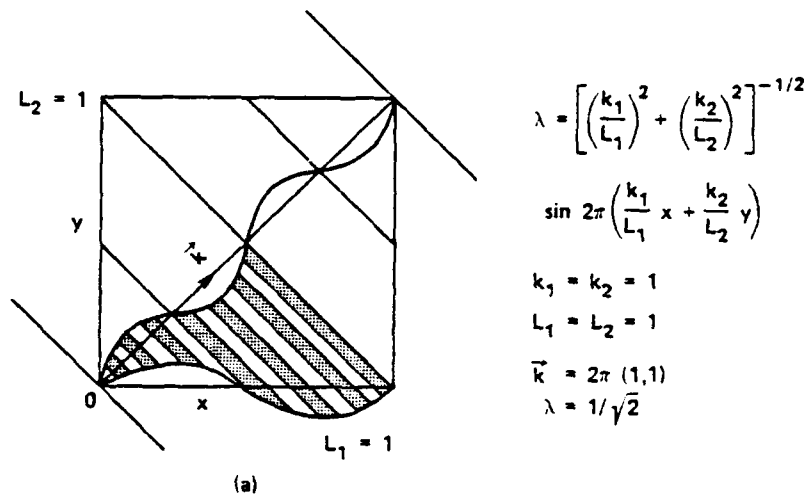


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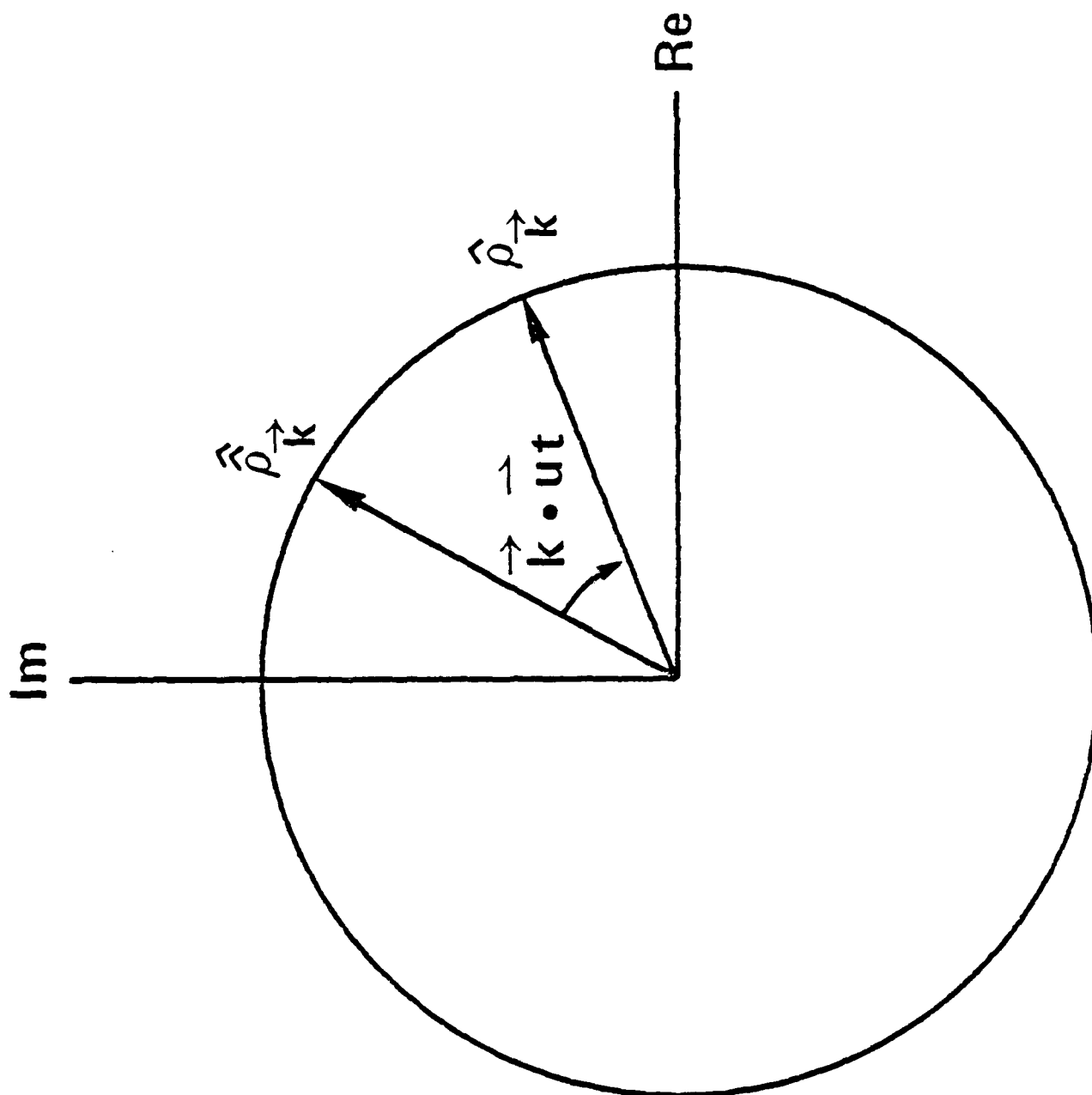


Fig. 22

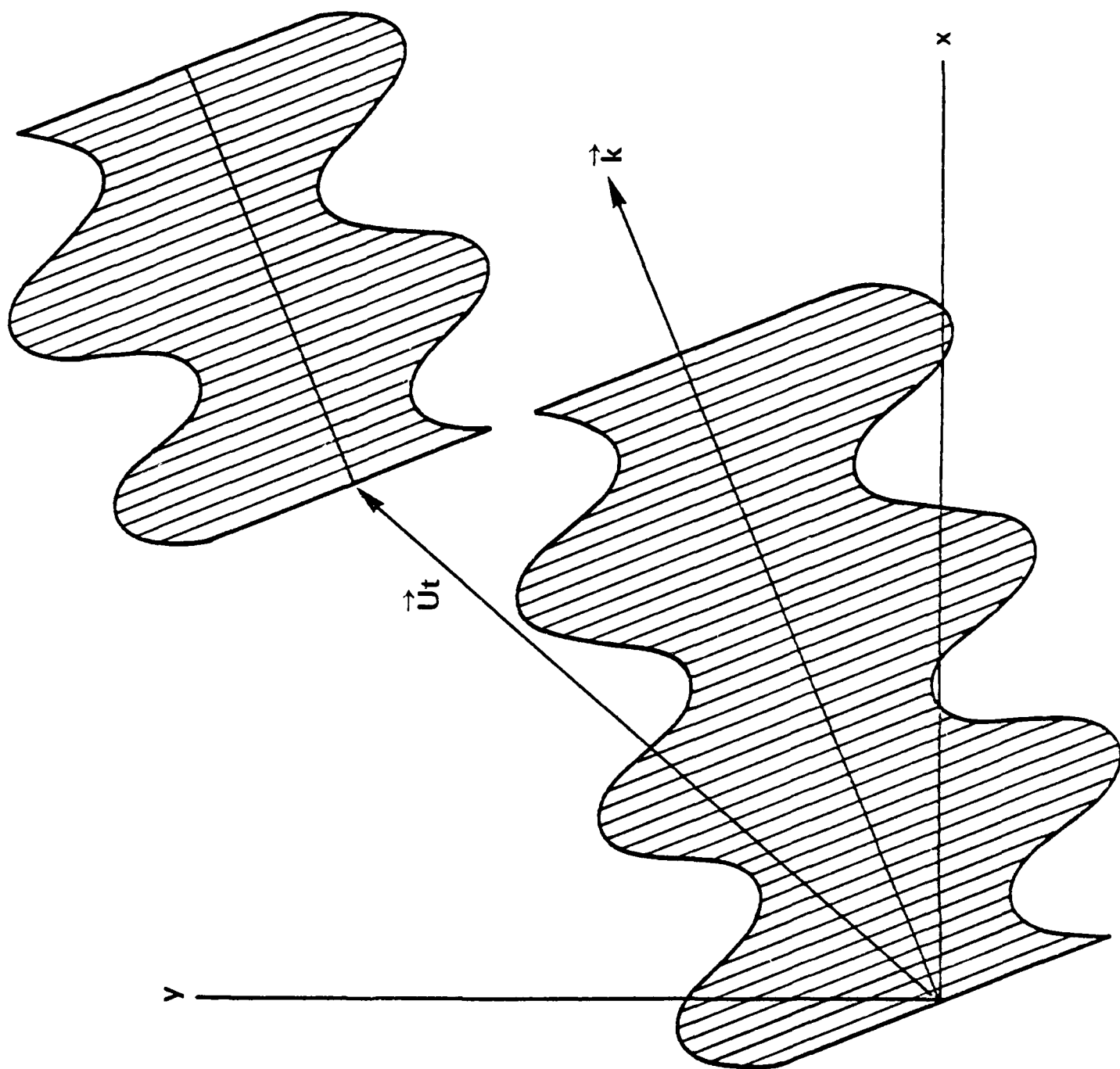


Fig. 23

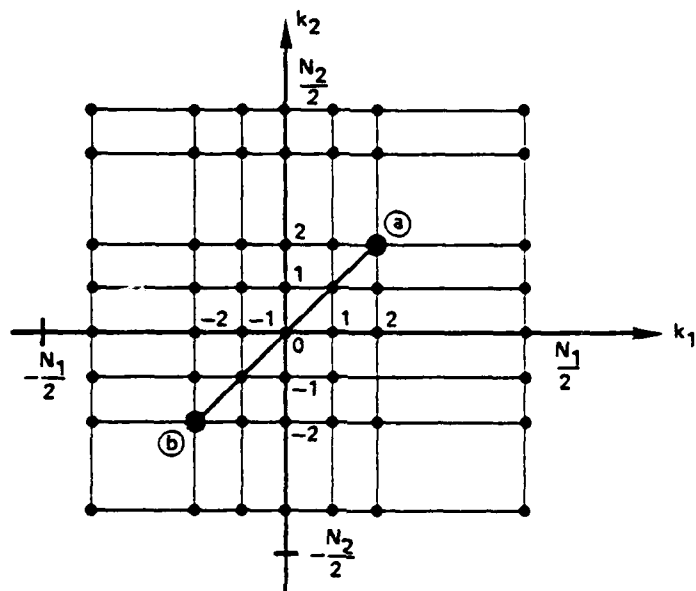


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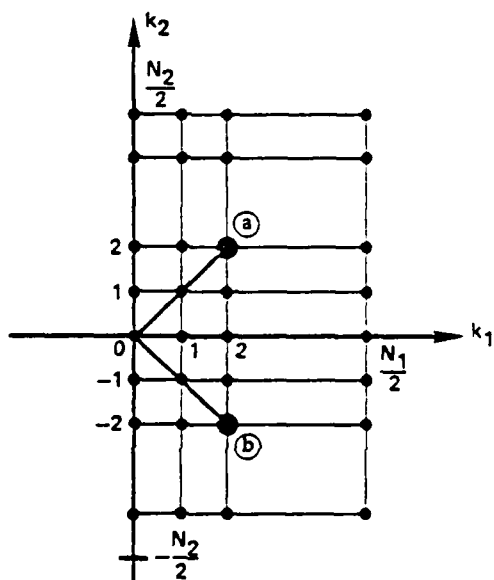


Fig. 25

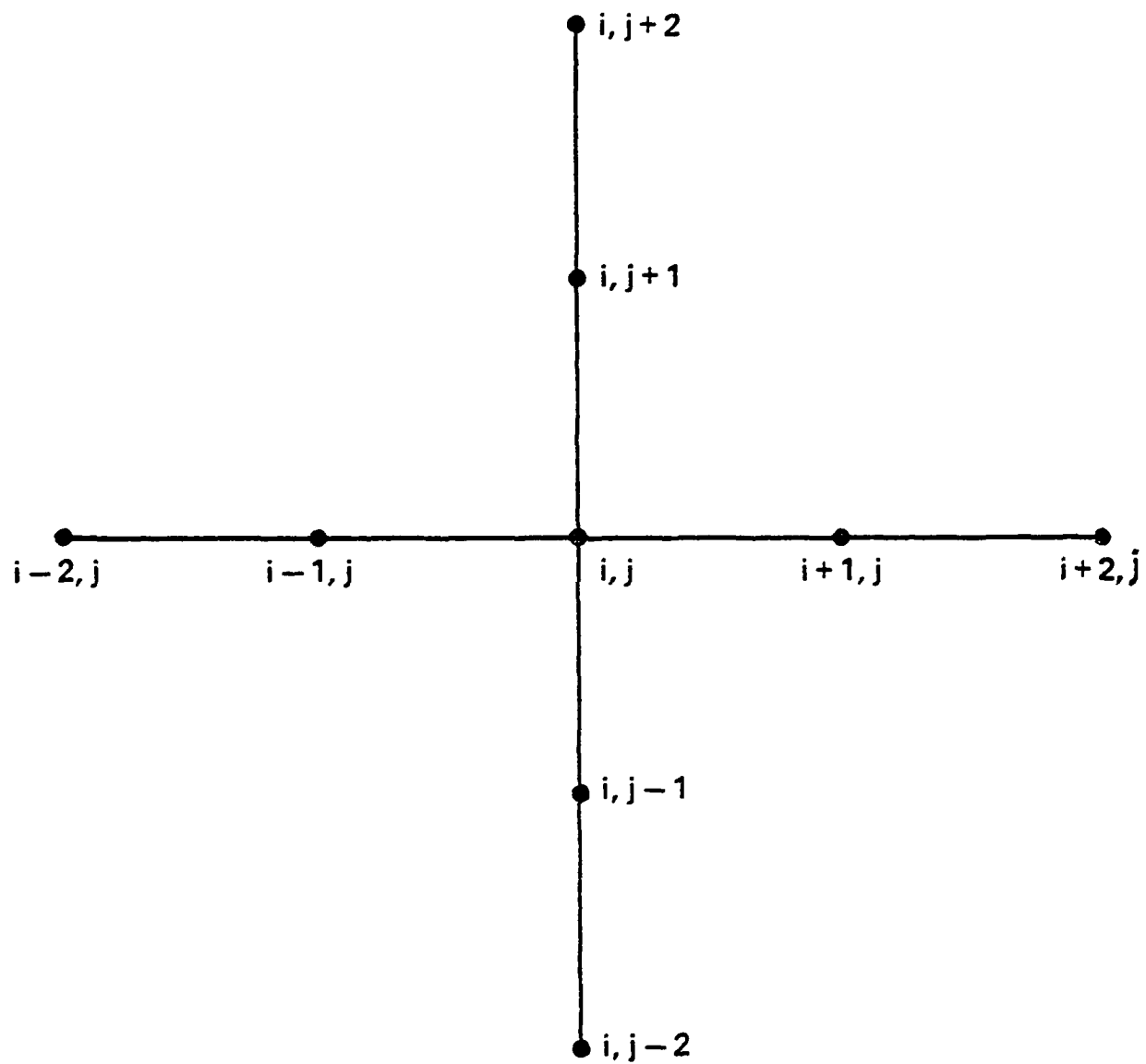


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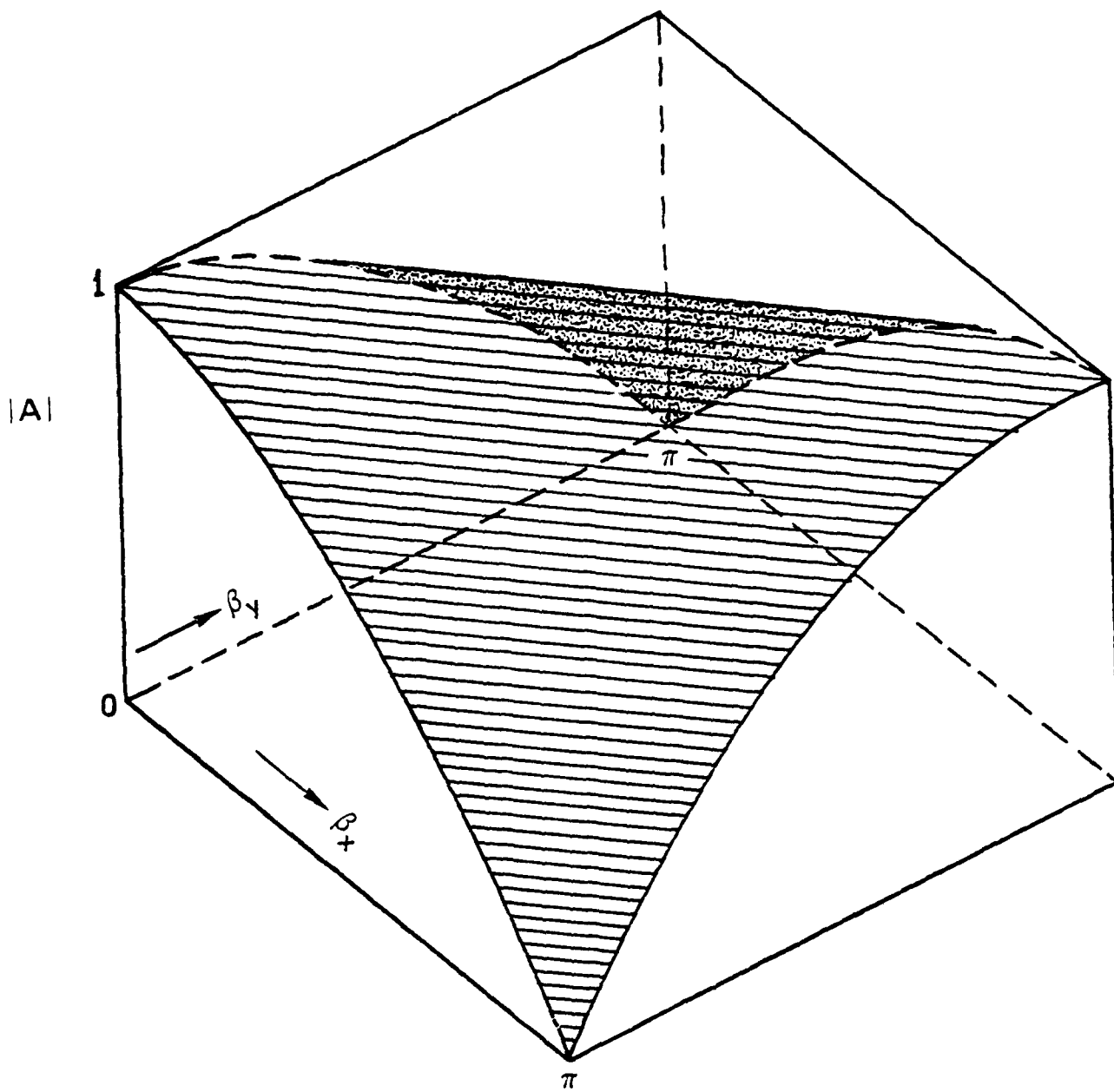


Fig. 27



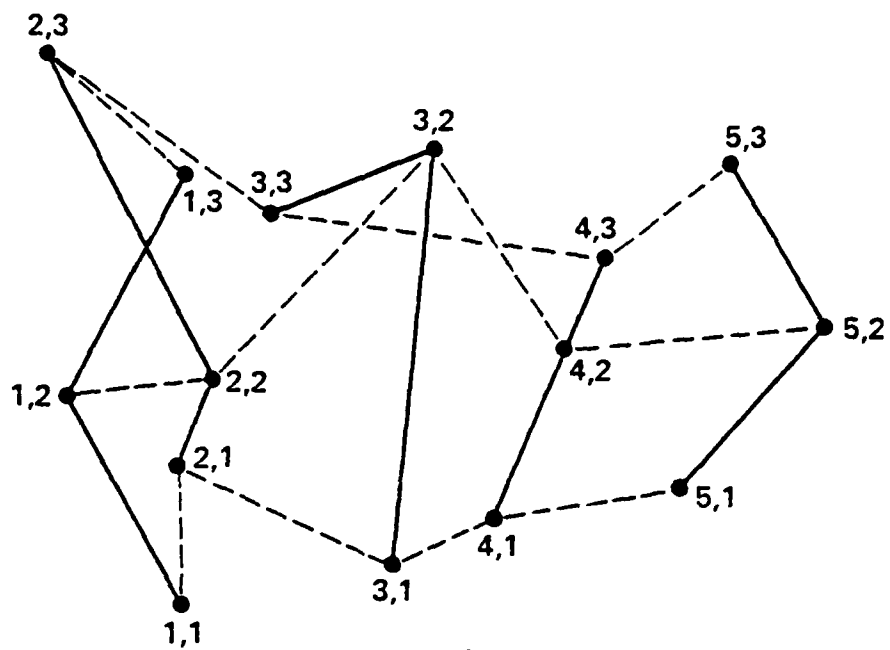


Fig. 28

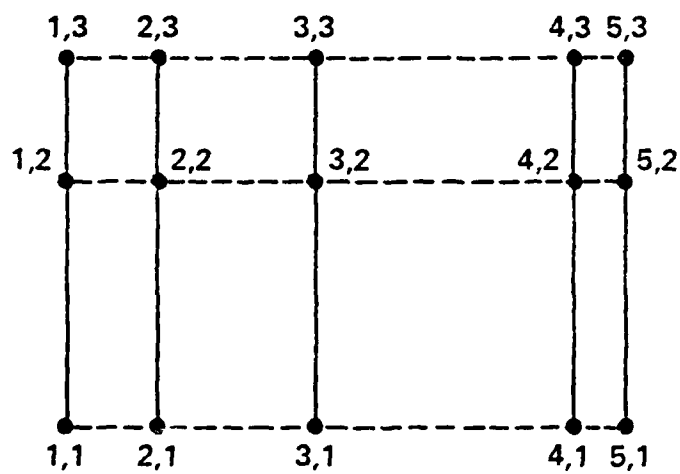


Fig. 29

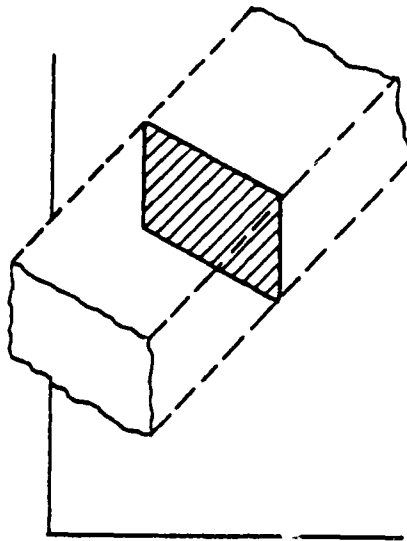


Fig. 30-1

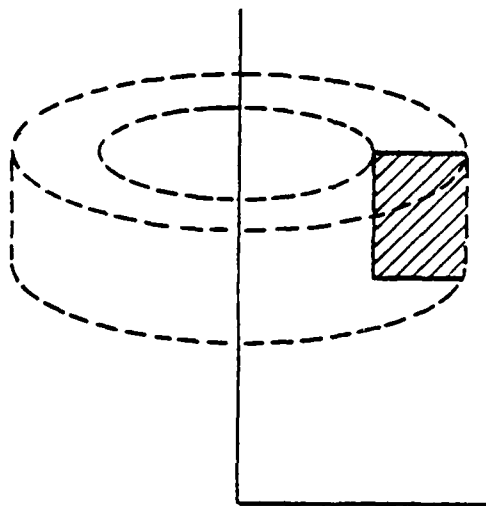


Fig. 30-2

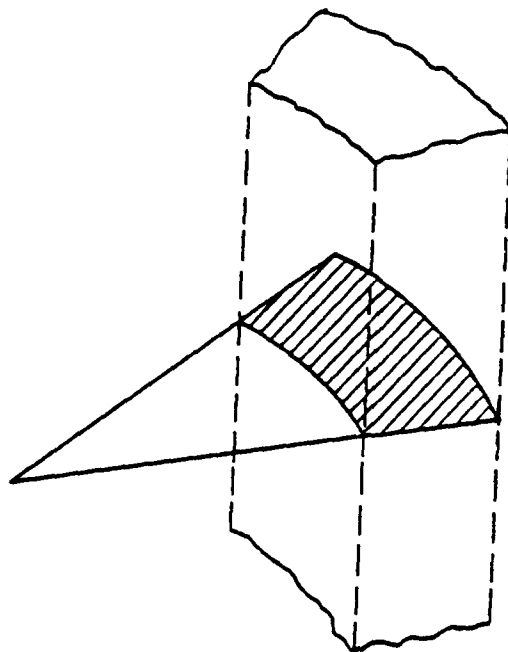


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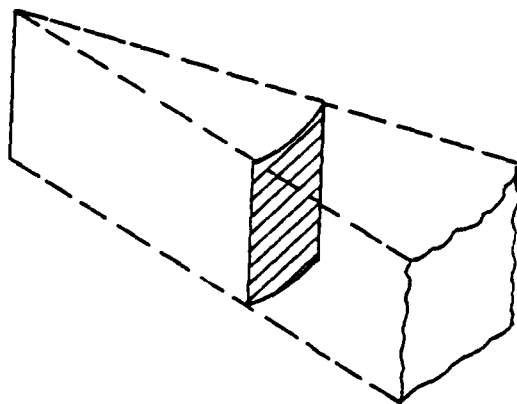


Fig. 30-4

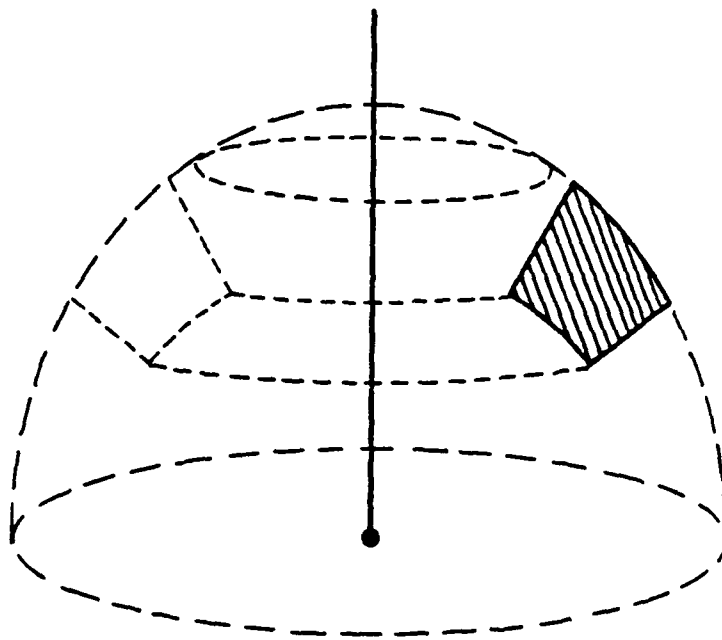


Fig. 30-5

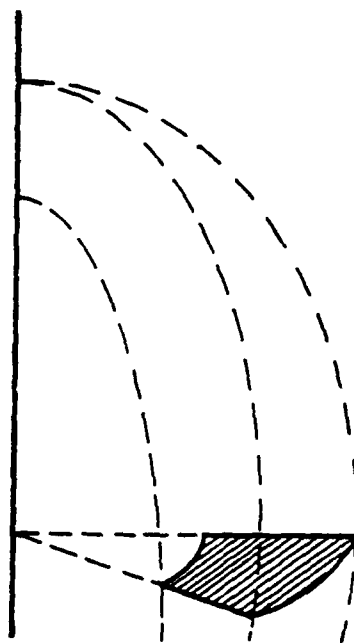


Fig. 30-6

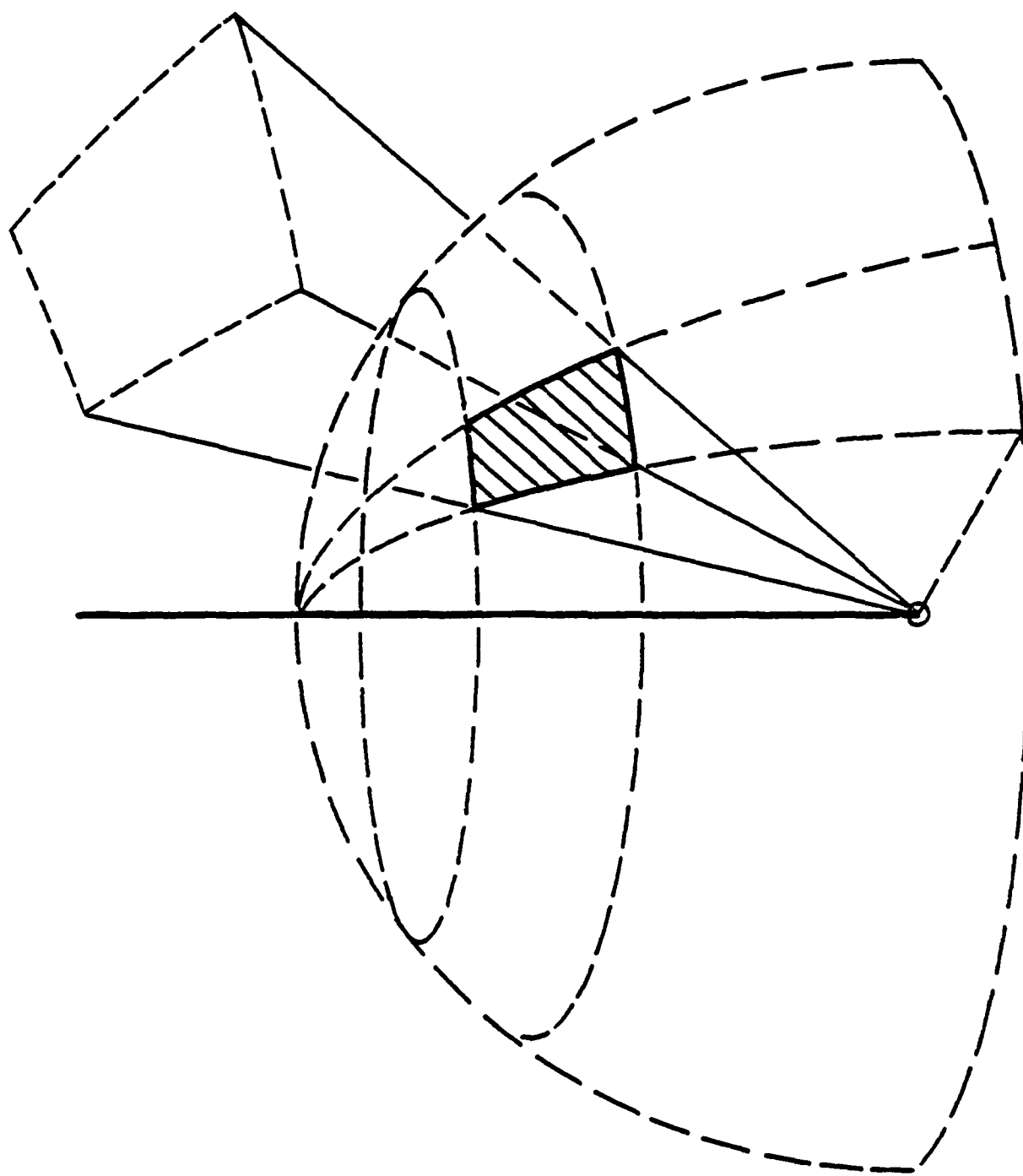


Fig. 33-7

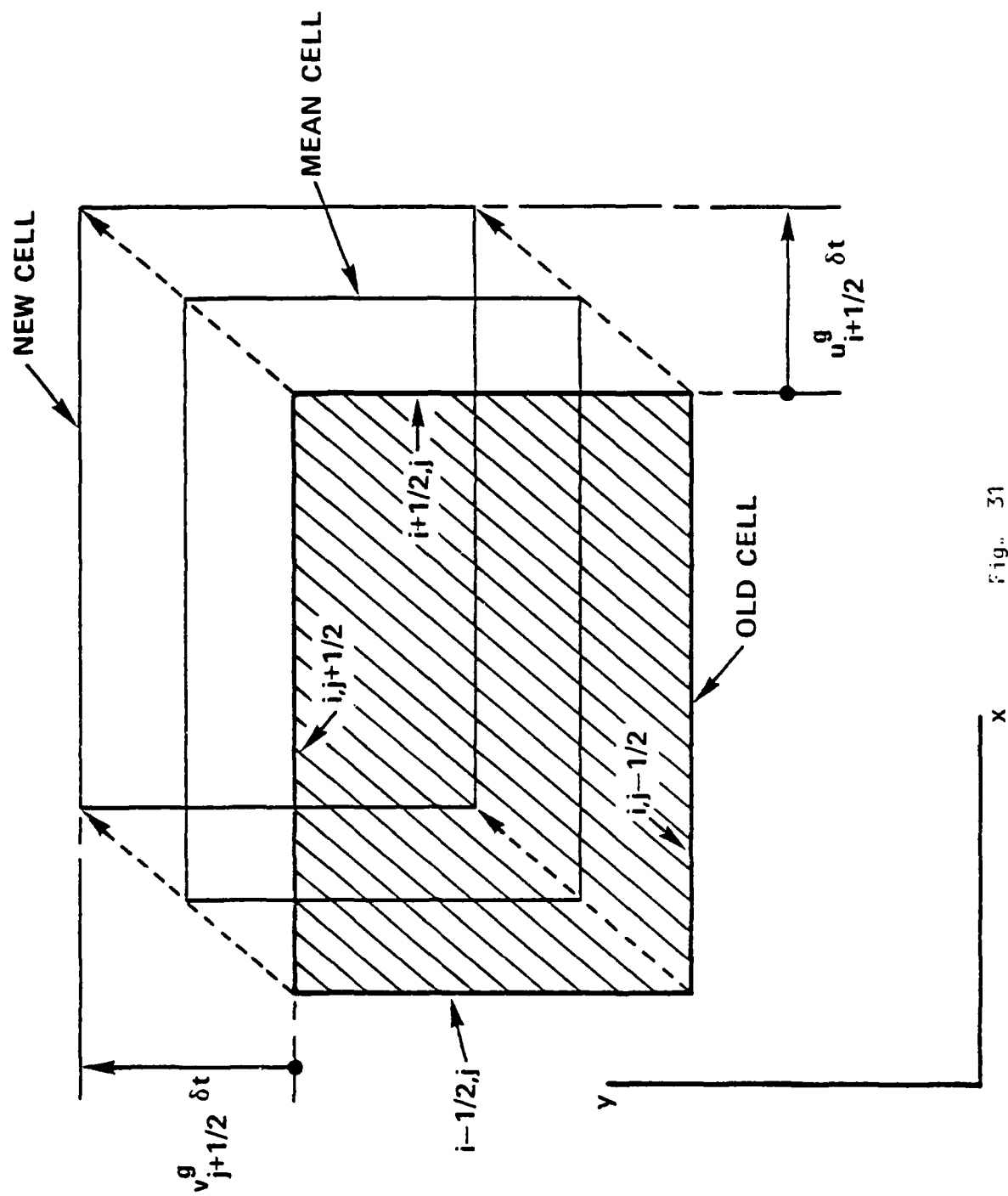


Fig. 31

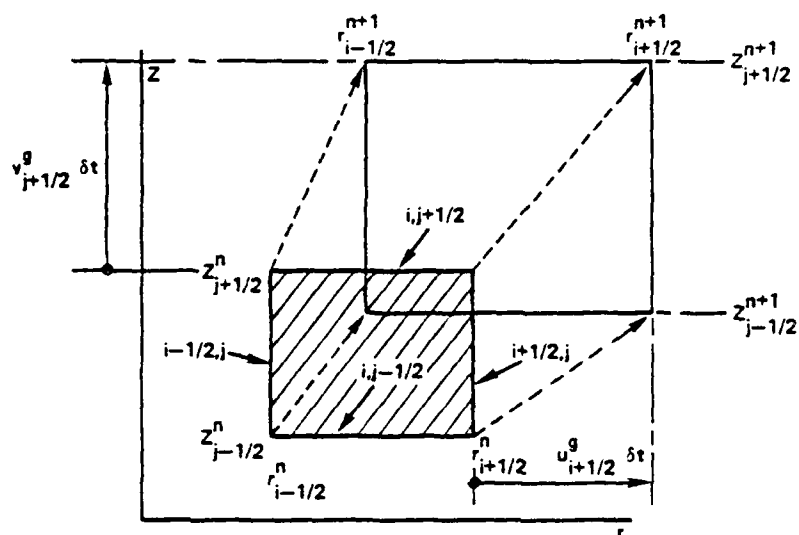


Fig. 52

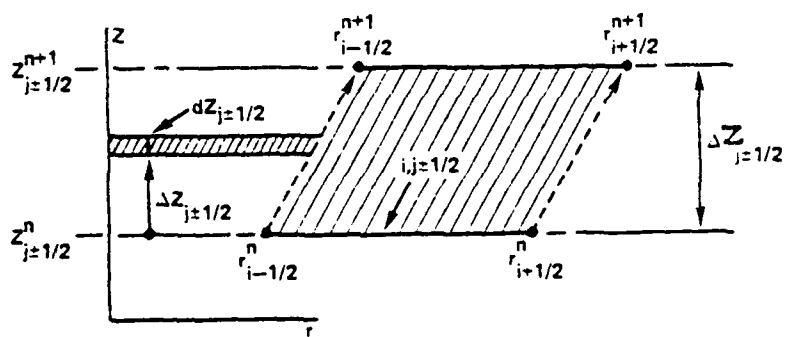


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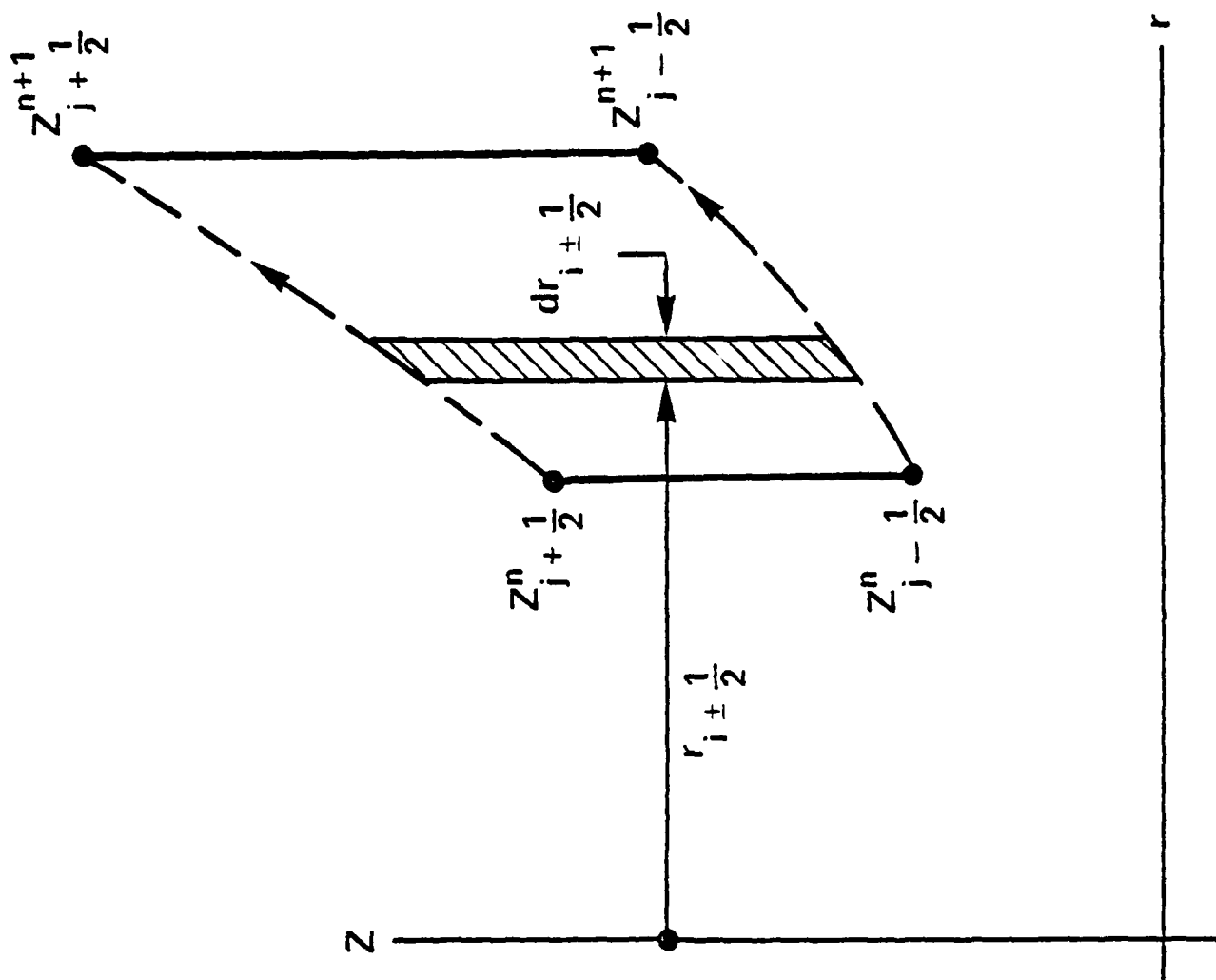


Fig. 34



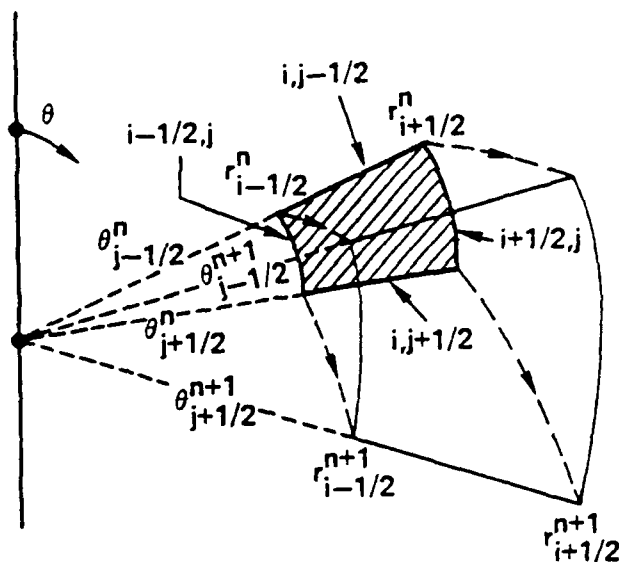


Fig. 35

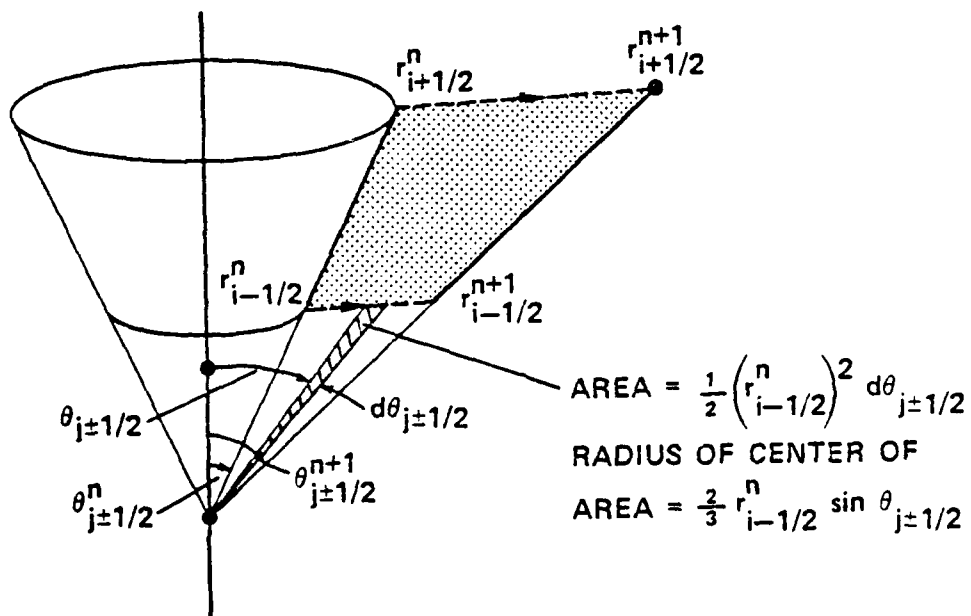


Fig. 36

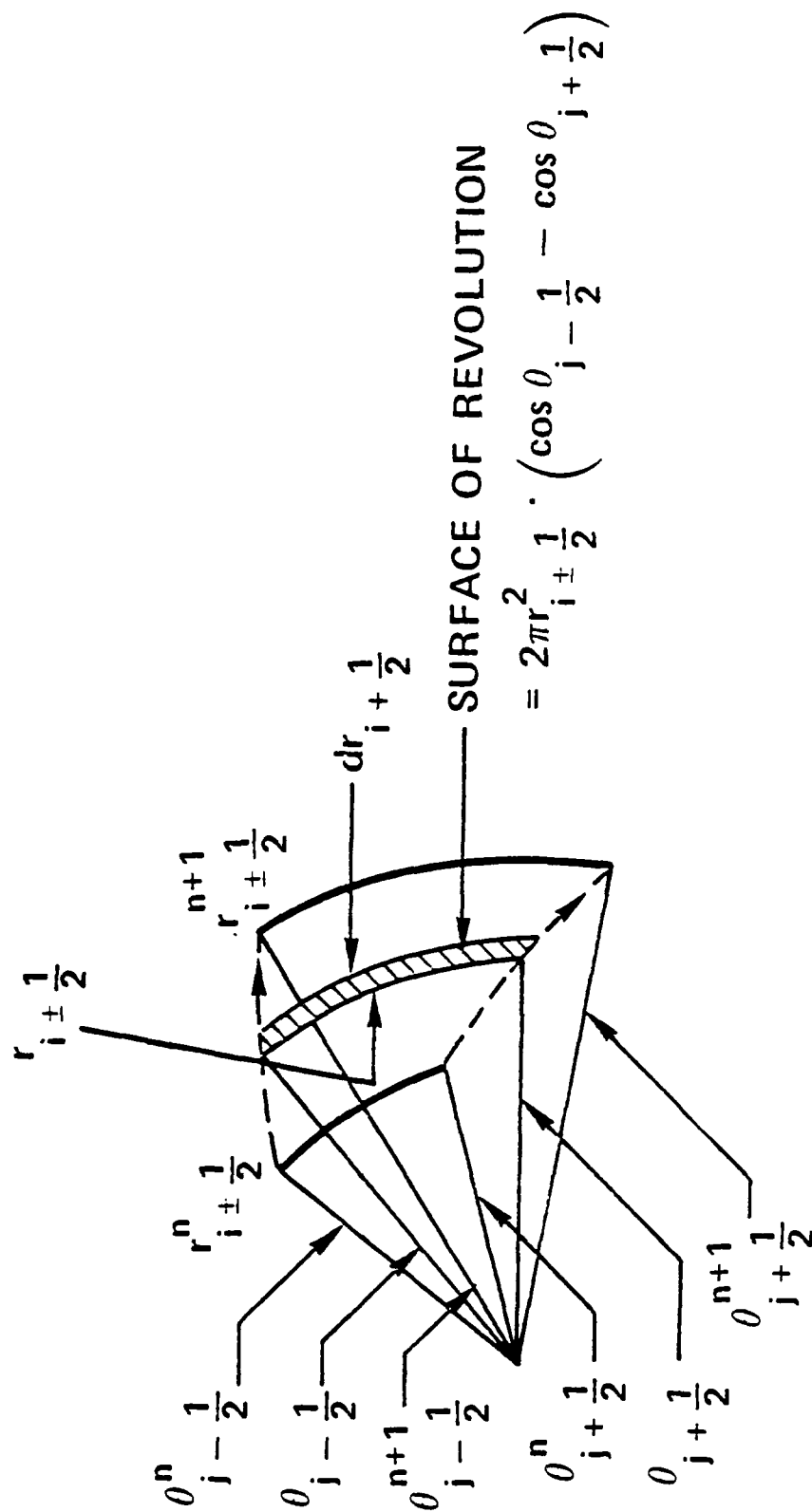


Fig. 37

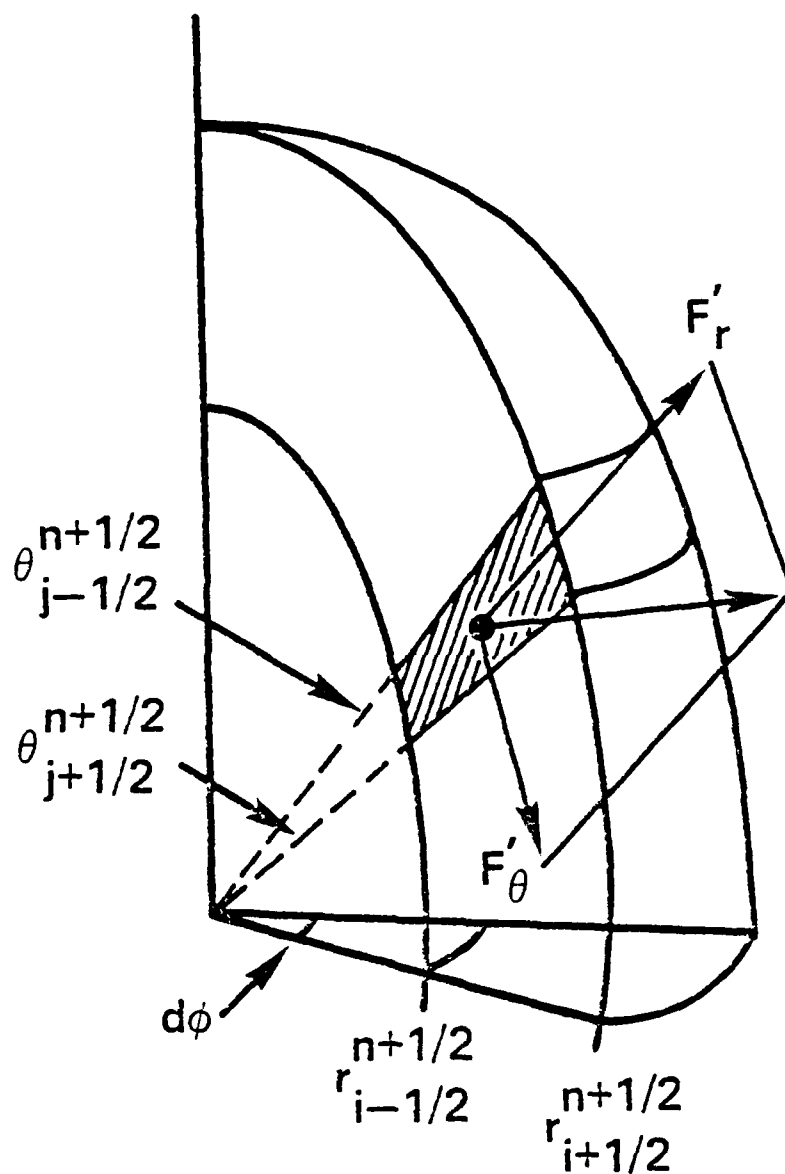


Fig. 30

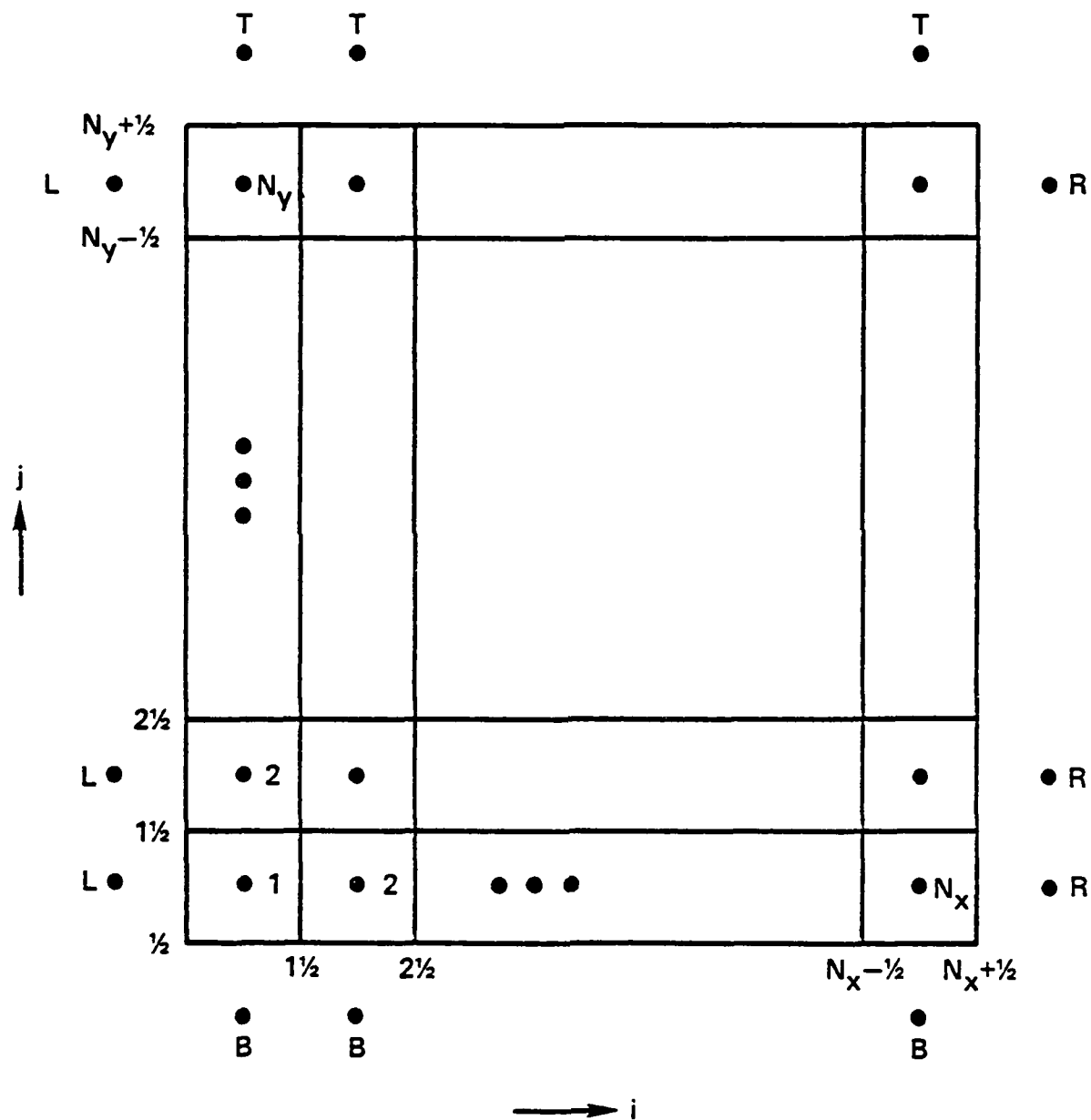


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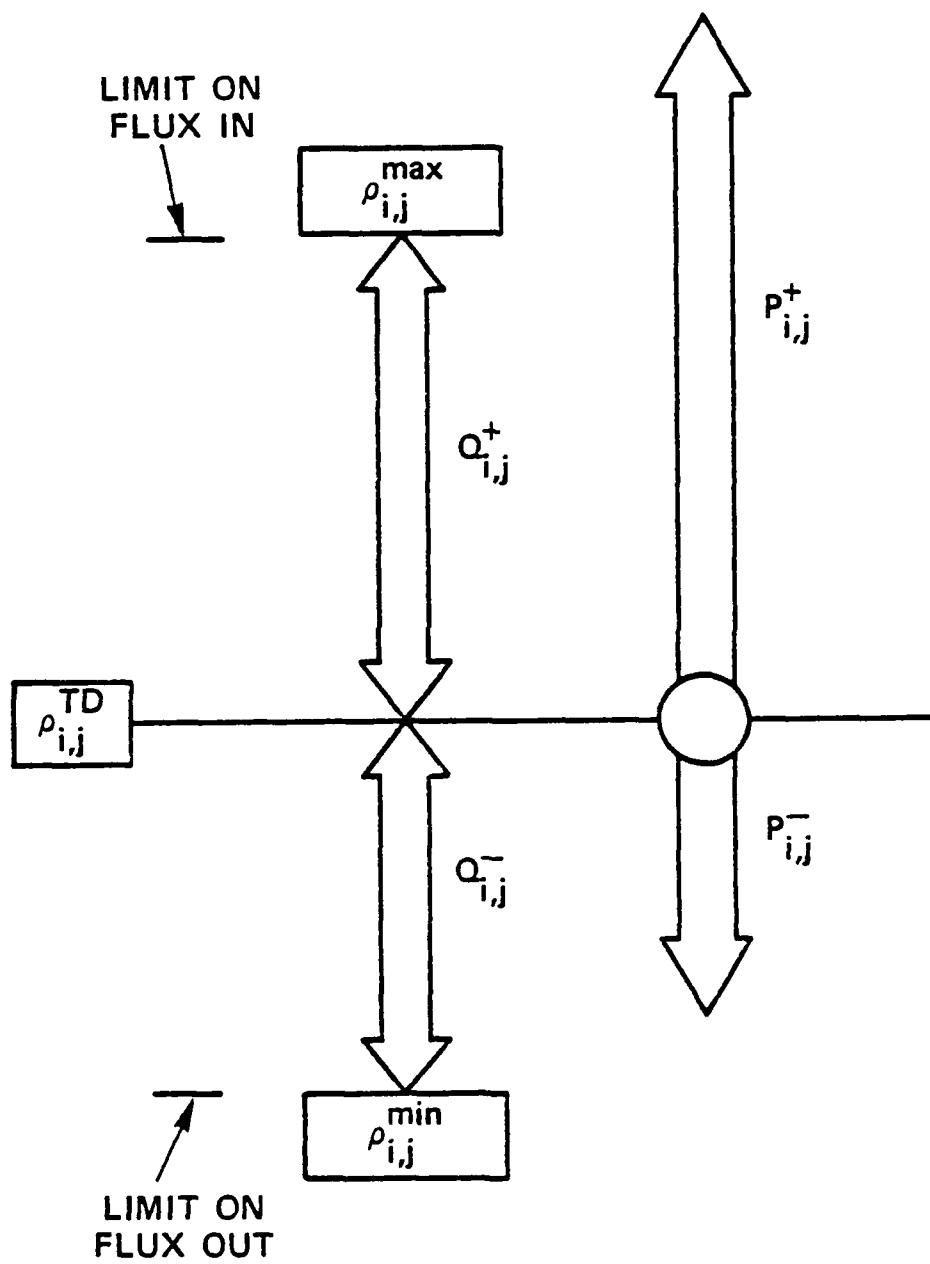


Fig. 40

*APPENDIX*

SUBROUTINE FCT2D(RHO,KO,KN,KR,SNKRNZ,  
& LBC,RHOLBC,RBC,RHORBC,BBC,RHOBBC,TBC,RHOTBC)

ORIGINATOR : RAAFAT H. GUIRGUIS

DESCRIPTION :

-----  
A FULLY 2-D ROUTINE THAT SOLVES GENERALIZED CONTINUITY EQUATIONS  
OF THE FORM

$$\partial \text{RHO} / \partial T = - \text{DIV}(\text{RHO} * \text{V}) - \text{SOURCES}$$

WHERE RHO IS THE GENERALIZED DENSITY, AND V IS THE FLUID VELOCITY.  
FOR SECOND ORDER ACCURACY, IT IS ADVISABLE TO ADVANCE HALF A  
TIME STEP USING THE VELOCITY AND SOURCE TERMS AT THE BEGINNING  
OF THE TIME STEP, THEN ADVANCE A WHOLE TIME STEP USING THE  
HALF-POINT VELOCITY AND SOURCE TERMS. USING THE HALF POINT  
DENSITY IS NOT RECOMMENDED. IT IS, HOWEVER, INCLUDED AS AN  
OPTION, BY ALTERNATING (KO,KN) BETWEEN (1,2) FOR THE HALF TIME  
STEP, AND (2,1) FOR THE WHOLE TIME STEP.  
THE OLD, (KO), AND NEW, (KN), DENSITIES ( AT THE BEGINNING AND END  
OF THE TIME STEP, RESPECTIVELY ) ARE STORED IN A 2-LEVEL 2-D ARRAY  
( 3-D ARRAY ). THE MASS AND DIFFUSION FLUXES ARE EVALUATED USING  
KO DENSITY, WHEREAS KN DENSITY DETERMINES THE ANTI-DIFFUSION  
FLUXES. IT IS ADVISABLE TO SET KO = 1, KN = 2, UNLESS THE HALF  
POINT DENSITY IS TO BE USED DURING THE WHOLE TIME STEP. THEN  
KO = 2, KN = 1 FOR THE WHOLE TIME STEP.  
KR DETERMINES THE LOCATION OF THE RESULTING DENSITY. IT IS  
ADVISABLE TO SET KR = 2 , 1 , FOR THE HALF AND WHOLE TIME STEPS,  
RESPECTIVELY. THIS CHOICE ELIMINATES THE NEED TO COPY THE NEW  
DENSITY ON THE OLD ARRAY, IN PREPARATION FOR A NEW TIME STEP.  
SNKRNZ IS A LOGICAL VARIABLE WHICH, WHEN SET TO .TRUE., TELLS THE  
ROUTINE TO USE THE CORRECTION FACTORS OF THE LAST SNKRNZ = .FALSE.  
CALL, TO LIMIT THE ANTI-DIFFUSION FLUXES. IF SET TO .FALSE., THE  
CORRECTION FACTORS ARE EVALUATED FROM THE CURRENT VARIABLES AND  
USED IN THE LIMITING PROCESS.  
LBC, RHOLBC, RBC, RHORBC, BBC, RHOBBC, TBC, RHOTBC, ARE DEFINED  
BELOW.

- (1) A PARTICULAR GEOMETRY IS SELECTED BY A CALL TO ENTRY  
SETGOM :  
CALL SETGOM( 4HCART, 1HX, 1HY, NX, NY )  
OR ...1HX, 1HZ,... OR ..., 1HZ, 1HY,..., ASSUMES CARTESIAN  
COORDINATES. ORDER OF THE 2 COORDINATES IS IMMATERIAL ONLY  
FOR THIS CASE.  
CALL SETGOM( 3HCYL, 1HR, 1HZ, NX, NY )  
CALL SETGOM( 3HCYL, 1HR, 3HFYE, NX, NY )  
CALL SETGOM( 3HCYL, 1HZ, 3HFYE, NX, NY )  
FOR THE 3 TYPICAL CYLINDRICAL COORDINATES.  
CALL SETGOM( 3HSPH, 1HR, 4HCETA, NX, NY )

CALL SETGOM( 3HSPH, 1HR, 3HFYE, NX, NY )  
 CALL SETGOM( 3HSPH, 4HCETA, 3HFYE, NX, NY )  
 FOR THE 3 TYPICAL SPHERICAL COORDINATES.  
 NX, NY, ARE THE NUMBERS OF CELLS CENTERS ALONG THE 2  
 COORDINATES, IN THE PRESCRIBED ORDER. IF THE LITERAL  
 CONSTANTS DESCRIBING THE GEOMETRY ARE MISS-SPELLED, AN ERROR  
 MESSAGE IS ISSUED, AND EXECUTION STOPPED.  
 NOTE : THE 2 COORDINATES ARE GENERALLY DENOTED BY (X,Y). IN  
 SPHERICAL R-FYE GEOMETRY, FOR EXAMPLE, X MEANS R, WHILE  
 Y MEANS FYE.

- (2) THE LEFT, RIGHT, BOTTOM, AND TOP BOUNDARIES ARE EXTENDED  
 1 CELL BEYOND THE LAST GRID POINT, YIELDING  $(NX+2)*(NY+2)$   
 CELLS. THE DENSITY OF AN EXTRA LEFT CELL = LBC \* (DENSITY  
 OF ADJACENT CELL ON SAME ROW) + RHOLBC. BY ADJUSTING THE  
 VALUES OF THE TWO 1-D REAL ARRAYS ( OF DIMENSION  $NY+2$  ) LBC  
 AND RHOLBC, VARIOUS TYPES OF BOUNDARIES CAN BE SIMULATED.  
 SIMILAR RELATIONS APPLY FOR RIGHT, BOTTOM, AND TOP  
 BOUNDARIES, DENOTED BY R, B, AND T, RESPECTIVELY. NOTE  
 THAT BOTTOM AND TOP ARRAYS ARE  $NX+2$  CELLS LONG.

- (3) ALL THE BOUNDARIES ARE CONSIDERED PERMEABLE TO DIFFUSION AND  
 ANTI-DIFFUSION FLUXES, UNLESS A CALL TO ENTRY SOLDFY INFORMS  
 THE ROUTINE OTHERWISE. ANY OF  
 CALL SOLDFY( 4HLEFT, KSTRT, KEND )  
 CALL SOLDFY( 4HRITE, KSTRT, KEND )  
 CALL SOLDFY( 4HBOTM, KSTRT, KEND )  
 CALL SOLDFY( 3HTOP, KSTRT, KEND )  
 MAKES THE LEFT, RIGHT, BOTTOM, OR TOP BOUNDARIES IMPERMEABLE  
 TO BOTH DIFFUSION AND ANTI-DIFFUSION FLUXES FROM CELL  
 NUMBER KSTRT TO CELL NUMBER KEND, INCLUSIVE.  
 NOTE : CELL 1 IS NOW THE EXTRA CELL BEYOND THE BOUNDARY,  
 CONFINING CELLS 2 TO  $NX+1$ , OR  $NY+1$ .  
 ANY NUMBER OF CALLS TO SOLDFY IS ALLOWED, MAKING  
 IT POSSIBLE TO SOLIDIFY UNCONNECTED PATCHES ALONG EACH  
 BOUNDARY. EACH TIME SOLDFY IS CALLED, A MESSAGE EXPLAINING  
 THE ACTION TAKEN IS ISSUED.

- (4) CALLS TO ENTRY PRODIC, FOR EXAMPLE,  
 CALL PRODIC( 1 , 1HX )  
 INFORM THE ROUTINE TO TREAT THE 1 ST OR 2 ND COORDINATE AS  
 PERIODIC. THE SECOND ARGUMENT IS JUST TO GENERATE A LABEL;  
 THE MESSAGE " X COORDINATE PERIODIC " IS ISSUED. SIMILARLY,  
 CALL PRODIC( 2 , 3HFYE )  
 MAKES THE 2 ND COORDINATE PERIODIC, AND THE MESSAGE " FYE  
 COORDINATE PERIODIC " ISSUED.  
 IF THE PERIODIC CALL IS MADE FOR A COORDINATE THAT SHOULDN'T  
 BE PERIODIC, A WARNING MESSAGE IS ISSUED, THEN EXECUTION  
 PROCEEDS.



C (5) THE GRID IS INITIALIZED BY A CALL TO ENTRY ORIGRD:  
 C CALL ORIGRD( XGN, YGN )  
 C WHERE XGN, YGN ARE TWO 1-D REAL ARRAYS OF DIMENSIONS NX+1,  
 C NY+1, CONTAINING THE LOCATIONS OF X, Y INTERFACES.  
 C ORIGRD WILL THEN CONSIDER THESE AS THE INITIAL LOCATIONS.  
 C AT THE BEGINNING OF EACH TIME STEP  
 C CALL NGRID( XGN, YGN )  
 C WILL EVALUATE VOLUME, MEAN INTERFACE AREA,... OF CELLS,  
 C WHEREAS  
 C CALL OGRID( XGN, YGN )  
 C AT THE END OF EACH TIME STEP, RESET THE OLD ARRAYS  
 C FOR THE NEXT TIME STEP.  
 C  
 C (6) IT IS ASSUMED THAT THE GRID IS MOVING, UNLESS CALLS TO ENTRY  
 C FIXGRD FIX ONE OR BOTH OF THE COORDINATES GRIDS.  
 C CALL FIXGRD( 1 , 1HX )  
 C INFORMS THE ROUTINE THAT THE 1 ST COORDINATE GRID IS FIXED.  
 C THE SECOND ARGUMENT IS JUST TO GENERATE A LABEL; THE MESSAGE  
 C "X GRID FIXED " IS ISSUED. SIMILARLY,  
 C CALL FIXGRD( 2 , 1HZ )  
 C FIXES THE 2 ND COORDINATE GRID AND ISSUES THE MESSAGE " Z  
 C GRID FIXED ". IF BOTH COORDINATES GRIDS ARE FIXED, CALL  
 C NGRID, THEN OGRID, ONLY ONCE AFTER INITIALIZATION.  
 C  
 C (7) A PARTICULAR ANTI-DIFFUSION FLUX CORRECTOR IS SELECTED BY A  
 C CALL TO ENTRY SETLMT :  
 C CALL SETLMT( 5HBORIS, 4HBOOK )  
 C INVOKES BORIS-BOOK FLUX LIMITER, WHILE  
 C CALL SETLMT( 7HZALESASAK, 1H )  
 C INVOKES ZALESASAK FLUX LIMITER. THE ARGUMENTS REFER TO THE  
 C ORIGINATORS OF THE FLUX LIMITER. IF THE LITERAL CONSTANTS  
 C DESCRIBING A LIMITER ARE MISS-SPELLED, AN ERROR MESSAGE IS  
 C ISSUED, AND EXECUTION STOPPED.  
 C  
 C (8) A TIME STEP STARTS BY A CALL TO ENTRY NGRID, FOLLOWED BY  
 C CALL VOLFLX( U, V, DT )  
 C WHERE U,V ARE TWO 2-D REAL ARRAYS OF DIMENSIONS (NX+2)\*(NY+2)  
 C CONTAINING THE COMPONENTS OF VELOCITY VECTOR AT THE CELLS  
 C CENTERS. DT IS THE TIME STEP.  
 C  
 C (9) BEFORE EACH CALL TO FCT2D, THE SOURCE TERM IS DETERMINED  
 C BY A SEQUENCE OF CALLS :  
 C CALL CLRSRC  
 C CLEARS THE SOURCE TERM WHICH REMAINS ZERO UNTIL ANY OF THE  
 C NEXT CALLS IS DONE. EACH CALL ADDS TO THE SOURCE TERM.  
 C ANY NUMBER OF CALLS IS ALLOWED, TO FORM THE TOTAL VALUE OF  
 C THE SOURCE TERM.  
 C CALL SRCES( 3HBDF, SRCOE, DT )  
 C ADDS A BODY TYPE FORCE, WHERE SRCOE IS A 2-D REAL ARRAY OF  
 C DIMENSION (NX+2)\*(NY+2) CONTAINING THE BODY FORCES PER UNIT  
 C VOLUME.

```

C      CALL SORCES( 4HXGRD, SORCE, DT )
C      CALL SORCES( 4HYGRD, SORCE, DT )
C      ADDS THE X OR Y COMPONENTS OF THE GRADIENT OF THE QUANTITY
C      IN ARRAY SORCE.
C      CALL SORCES( 3HDIV, SORCE, DT )
C      ADDS THE DIVERGENCE OF THE QUANTITY IN SORCE.  ENTRY SORCES
C      DETERMINES WHICH FORM OF GRADIENT OR DIVERGENCE TO USE
C      ACCORDING TO THE GEOMETRY.  ALTERNATIVELY, ONE CAN
C      SEPARATELY CALL ENTRY BODY FOR BODY FORCES, XGRAD OR YGRAD
C      FOR THE GRADIENT IN CARTESIAN COORDINATES, RCGRAD OR YGRAD
C      FOR THE GRADIENT IN CYLINDRICAL R-Z GEOMETRY,... OR XGRAD AND
C      YGRAD FOR DIVERGENCE IN CARTESIAN GEOMETRY, RCDIV AND YGRAD
C      DIVERGENCE IN CYLINDRICAL R-Z GEOMETRY,...
C
C      (10) THE TIME STEP ENDS BY A CALL TO OGRID
C
C      (11) FOR 2 ND ORDER ACCURACY, STEPS (8) , (9) ARE PERFORMED TWICE.
C      ONCE WITH DT= TIME STEP / 2 FOR THE HALF TIME STEP, THEN
C      DT= TIME STEP FOR THE WHOLE TIME STEP.
C
C      ENTRIES ...
C      ENTRY NGRID(XGN,YGN)
C      ENTRY OGRID(XGN,YGN)
C      ENTRY ORIGRD(XGN,YGN)
C      ENTRY VOLFLX(U,V,DT)
C      ENTRY SORCES(SRCTYP,SORCE,DT)
C      ENTRY CLRSRC
C      ENTRY BODY(SORCE,DT)
C      ENTRY XGRAD(SORCE,DT)
C      ENTRY YGRAD(SORCE,DT)
C      ENTRY RCGRAD(SORCE,DT)
C      ENTRY RCDIV(SORCE,DT)
C      ENTRY SETGOM(GOMTRY,CRD1,CRD2,N1,N2)
C      ENTRY PRODIC(CRDNT,CRD)
C      ENTRY SETLMT(LMTR1,LMTR2)
C      ENTRY FIXGRD(CRNT,CRD)
C      ENTRY SOLDFY(BONDRY,KSTRT,KEND)
C
C      CALLS TO ...
C      SUBROUTINE NUMU(NI,NJ,EPS,NUV,MUV)
C

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C      DECLARATIONS :
C      -----
C
C      PARAMETER      NPX=100,NPY=100
C      PARAMETER      NP1X=NPX+1,NP1Y=NPY+1
C      PARAMETER      NP2X=NPX+2,NP2Y=NPY+2
C
C
C      INTEGER      GEOM,CORNT
C
C      INTEGER      IFLX(NP2X,NP2Y)
C
C
C      LOGICAL      LSRC
C      LOGICAL      SNKRNZ
C      LOGICAL      XCHNG,YCHNG
C      LOGICAL      XPRDC,YPRDC
C
C
C      REAL      TEXT(20)
C      REAL      LMTR1(2),LMTR2(2)
C      REAL      TGM(3),TCRD(6),TLM1(2,4),TLM2(2,4)
C
C      REAL      LBC(NP2Y),RHQLBC(NP2Y)
C      REAL      RBC(NP2Y),RHQRBC(NP2Y)
C      REAL      BBC(NP2X),RHQBBC(NP2X)
C      REAL      TBC(NP2X),RHQTBC(NP2X)
C
C      REAL      PRMBLL(NP2Y),PRMBLR(NP2Y),PRMELB(NP2X),PRMBLT(NP2X)
C
C      REAL      XGO(NP1X),XGN(NP1X),YGO(NP1Y),YGN(NP1Y)
C      REAL      XG(NP1X),DXG(NP1X),YG(NP1Y),DYG(NP1Y)
C      REAL      DXGO(NP2X),DXGN(NP2X),DYGO(NP2Y),DYGN(NP2Y)
C      REAL      RDXGN(NP2X),RDYGN(NP2Y)
C      REAL      DXGNH(NP1X),RDXGNH(NP1X),DYGNH(NP1Y),RDYGNH(NP1Y)
C      REAL      AX(NPX),AY(NPY)
C      REAL      SQ(NP1X),SQO(NP1X),SQN(NP1X)
C
C      REAL      RHQ(NP2X,NP2Y,2)
C      REAL      U(NP2X,NP2Y),ADUDT(NP1X,NPY)
C      REAL      V(NP2X,NP2Y),ADVDT(NPX,NP1Y)
C      REAL      CELMAS(NPX,NPY),SOURCE(NP2X,NP2Y),SORCE(NP2X,NP2Y)
C
C      REAL      TEMP1(NP2X,NP2Y),TEMP2(NP2X,NP2Y)
C      REAL      TEMP3(NP1X,NP1Y),TEMP4(NP1X,NP1Y)
C      REAL      TEMP5(NP2X,NP2Y),TEMP6(NP2X,NP2Y)
C
C      REAL      QLDVOL(NP2X,NP2Y),RVOL(NP2X,NP2Y)
C      REAL      AVXVL(NP1X,NP1Y),RAVXVL(NP1X,NP1Y)
C      REAL      AVYVL(NP1X,NP1Y),RAVYVL(NP1X,NP1Y)
C
C      REAL      XMSFLX(NP1X,NP1Y),YMSFLX(NP1X,NP1Y)
C      REAL      XDFFLX(NP2X,NP2Y),YDFFLX(NP2X,NP2Y)
C      REAL      XNTFLX(NP1X,NP1Y),YNTFLX(NP1X,NP1Y)

```

REAL EPSX (NP1X,NP1Y),NUX (NP2X,NP2Y),MUX (NP2X,NP2Y)  
 REAL EPSY (NP1X,NP1Y),NUY (NP2X,NP2Y),MUY (NP2X,NP2Y)  
 REAL NUXVOL (NP2X,NP2Y),MUXVOL (NP2X,NP2Y)  
 REAL NUYVOL (NP2X,NP2Y),MUYVOL (NP2X,NP2Y)

C

REAL MXFLX (NP2X,NP2Y),MNFLX (NP2X,NP2Y)  
 REAL FLXIN (NP2X,NP2Y),FLXOUT (NP2X,NP2Y)  
 REAL RHOMX (NP2X,NP2Y),RHOMN (NP2X,NP2Y)  
 REAL MXIN (NP2X,NP2Y),MXOUT (NP2X,NP2Y)  
 REAL DIFF (NP2X,NP2Y),FLX (NP2X,NP2Y)

C

REAL RIN (NP2X,NP2Y),ROUT (NP2X,NP2Y)  
 REAL XFLXCR (NP2X,NP2Y),YFLXCR (NP2X,NP2Y)

C

C

EQUIVALENCE (TEMP1,FLXIN,RIN)  
 EQUIVALENCE (TEMP2,FLXOUT,ROUT)  
 EQUIVALENCE (TEMP3,XMSFLX,XNTFLX,AVXVL,RAVXVL,EPSX)  
 EQUIVALENCE (TEMP4,YMSFLX,YNTFLX,AVYVL,RAVYVL,EPSY)  
 EQUIVALENCE (TEMP5,XDFFLX,YDFFLX,NUX,NUXVOL,NUY,NUYVOL)  
 EQUIVALENCE (TEMP5,OLDVOL,RVOL,DIFF,MXFLX,FLX,IFLX)  
 EQUIVALENCE (TEMP6,SOURCE,MUX,MUXVOL,MUY,MUYVOL)  
 EQUIVALENCE (TEMP6,RHOMX,RHOMN,MXIN,MXOUT,MNFLX)  
 EQUIVALENCE (TEMP6,XFLXCR,YFLXCR)

C

C

DATA TEXT(1),TEXT(2),TEXT(3)/4H M,4HISS-,4HSPEL/  
 DATA TEXT(4),TEXT(5)/4HLING,4H OF /  
 DATA TEXT(9),TEXT(10),TEXT(11)/4H IDE,4HNTIF,4HIER /  
 DATA TEXT(12),TEXT(13),TEXT(14)/4H GE,4HOMET,4HRY /  
 DATA TEXT(15),TEXT(16),TEXT(17)/4HFLUX,4H LIM,4HITER/  
 DATA TEXT(18),TEXT(19),TEXT(20)/4HSOUR,4HCE T,4HYPE /

C

DATA TGM(1),TGM(2),TGM(3)/4HCART,4HCOYL ,4HSPH /

C

DATA TCRD(1),TCRD(2),TCRD(3)/4HX ,4HY ,4HZ /  
 DATA TCRD(4),TCRD(5),TCRD(6)/4HR ,4HCETA,4HFYE /

C

DATA TBND(1),TBND(2)/4HLEFT,4HRITE/  
 DATA TBND(3),TBND(4)/4HBOTM,4HTOP /

C

DATA LMTR1,LMTR2/4\*4H /  
 DATA TLM1(1,1),TLM1(2,1)/4HBORI,4HS /  
 DATA TLM2(1,1),TLM2(2,1)/4HBOOK,4H /  
 DATA TLM1(1,2),TLM1(2,2)/4HZALE,4HSAK /  
 DATA TLM2(1,2),TLM2(2,2)/4H ,4H /

C

DATA BDF/3HBDF/,XGRD,YGRD/4HXGRD,4HYGRD/,DIV/3HDIV/

C

C

C  
C  
C

FORMATS :

-----

10     FORMAT(///5X,7HWARNING,5X,11A4)  
20     FORMAT(///5X,7HWARNING,5X,A4,2X,22HSHOULD NOT BE PERIODIC)  
30     FORMAT(///5X,24HALL BOUNDARIES PERMEABLE)  
40     FORMAT(///5X,A4,2X,19HCOORDINATE PERIODIC)  
50     FORMAT(///5X,A4,2X,10HGRID FIXED)  
60     FORMAT(///5X,A4,2X,22HBOUNDARY SOLID BETWEEN,  
    &         2X,4HCELL,2X,I4,2X,3HAND,2X,I4)  
70     FORMAT(///5X,25HGOMETRY NOT INCLUDED YET)

C  
C

```

C      EVALUATE OLD CELL MASS "CELMAS"
        DO 110 J=1,NY
        DO 110 I=1,NX
        OLDVOL(I,J)=DXGO(I+1)*DYGO(J+1)
110      CELMAS(I,J)=RHO(I+1,J+1,1)*OLDVOL(I,J)
C
C      ADD SOURCE TERM "SOURCE" WHEN APPROPRIATE
        IF(.NOT.LSRC) GO TO 125
C
C
        DO 120 J=1,NY
        DO 120 I=1,NX
120      CELMAS(I,J)=CELMAS(I,J)-SOURCE(I,J)
C
125      CONTINUE
C
C
C      EVALUATE X-CONVECTION FLUX "XMSFLX"
        DO 130 J=1,NY
        DO 130 I=1,NXP1
        TEMP3(I,J)=RHO(I+1,J+1,KO)+RHO(I,J+1,KO)
        TEMP5(I,J)=0.5*ADUDT(I,J)
130      XMSFLX(I,J)=TEMP3(I,J)*TEMP5(I,J)
C
C      EVALUATE Y-CONVECTION FLUX "YMSFLX"
        DO 140 J=1,NYP1
        DO 140 I=1,NX
        TEMP4(I,J)=RHO(I+1,J+1,KO)+RHO(I+1,J,KO)
        TEMP6(I,J)=0.5*ADVDT(I,J)
140      YMSFLX(I,J)=TEMP4(I,J)*TEMP6(I,J)
C
C      EVALUATE X AND Y TRANSPORTED DENSITIES
        DO 150 J=1,NY
        DO 150 I=1,NX
        TEMP5(I,J)=XMSFLX(I,J)-XMSFLX(I+1,J)
        TEMP6(I,J)=YMSFLX(I,J)-YMSFLX(I,J+1)
        TEMP3(I,J)=CELMAS(I,J)+TEMP5(I,J)
        TEMP4(I,J)=CELMAS(I,J)+TEMP6(I,J)
        CELMAS(I,J)=TEMP3(I,J)+TEMP6(I,J)
        RVOL(I,J)=RDXGN(I+1)*RDYGN(J+1)
        RHO(I+1,J+1,KN)=TEMP3(I,J)*RVOL(I,J)
150      TEMP4(I,J)=TEMP4(I,J)*RVOL(I,J)
C
C      EVALUATE X-TRANSPORTED DENSITY AT LEFT AND RIGHT BOUNDARIES
        DO 170 J=2,NYP1
        RHO(1,J,KN)=LBC(J)*RHO(IL,J,KN)+RHOLEB(J)
170      RHO(NXP2,J,KN)=RBC(J)*RHO(IR,J,KN)+RHOREC(J)
C

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C      EVALUATE "EPSX"
        DO 180 J=1,NY
          DO 180 I=1,NXP1
            RAVXVL(I,J)=RDXGNH(I)*RDYGN(J+1)
180      EPSX(I,J)=RAVXVL(I,J)*ADUDT(I,J)
C
C      EVALUATE X DIFFUSION AND ANTI-DIFFUSION COEFFICIENTS "NUX", "MUX"
        CALL NUMU(NXP1,NY,EPSX,NUX,MUX)
C
C      CANCEL THE DIFFUSION AND ANTI-DIFFUSION X-FLUXES THROUGH SOLID
C      PORTIONS OF LEFT AND RIGHT BOUNDARIES
        DO 185 J=1,NY
          NUX(1,J)=NUX(1,J)*FRMBLL(J+1)
          MUX(1,J)=MUX(1,J)*FRMBLL(J+1)
          NUX(NXP1,J)=NUX(NXP1,J)*FRMBLR(J+1)
185      MUX(NXP1,J)=MUX(NXP1,J)*FRMBLR(J+1)
C
C      EVALUATE X DIFFUSION AND ANTI-DIFFUSION FLUXES "XDFFLX" , "XNTFLX"
        DO 190 J=1,NY
          DO 190 I=1,NXP1
            AVXVL(I,J)=DXGNH(I)*DYGN(J+1)
            NUXVOL(I,J)=NUX(I,J)*AVXVL(I,J)
            MUXVOL(I,J)=MUX(I,J)*AVXVL(I,J)
            TEMP3(I,J)=RHO(I+1,J+1,KO)-RHO(I,J+1,KO)
            XDFFLX(I,J)=NUXVOL(I,J)*TEMP3(I,J)
            TEMP3(I,J)=RHO(I+1,J+1,KN)-RHO(I,J+1,KN)
190      XNTFLX(I,J)=MUXVOL(I,J)*TEMP3(I,J)
C
C      ADD X-DIFFUSION TO "CELMAS"
        DO 200 J=1,NY
          DO 200 I=1,NX
            RHO(I+1,J+1,KN)=TEMP4(I,J)
            TEMP6(I,J)=XDFFLX(I+1,J)-XDFFLX(I,J)
200      CELMAS(I,J)=CELMAS(I,J)+TEMP6(I,J)
C
C      EVALUATE Y-TRANSPORTED DENSITY AT BOTTOM AND TOP BOUNDARIES
        DO 210 I=1,NXP2
          RHO(I,1,KN)=BBC(I)*RHO(I,JB,KN)+RHOBBC(I)
210      RHO(I,NYP2,KN)=TBC(I)*RHO(I,JT,KN)+RHOTBC(I)
C
C      EVALUATE "EPSY"
        DO 220 J=1,NYP1
          DO 220 I=1,NX
            RAVYVL(I,J)=RDXGN(I+1)*RDYGNH(J)
220      EPSY(I,J)=RAVYVL(I,J)*ADVDT(I,J)
C
C      EVALUATE Y DIFFUSION AND ANTI-DIFFUSION COEFFICIENTS "NUY", "MUY"
        CALL NUMU(NX,NYP1,EPSY,NUY,MUY)
C

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C      CANCEL THE DIFFUSION AND ANTI-DIFFUSION Y-FLUXES THROUGH SOLID
C      PORTIONS OF BOTTOM AND TOP BOUNDARIES
        DO 225 I=1,NX
          NUY(I,1)=NUY(I,1)*PRMBLB(I+1)
          MUY(I,1)=MUY(I,1)*PRMBLB(I+1)
          NUY(I,NYP1)=NUY(I,NYP1)*PRMBLT(I+1)
225      MUY(I,NYP1)=MUY(I,NYP1)*PRMBLT(I+1)
C
C      EVALUATE Y DIFFUSION AND ANTI-DIFFUSION FLUXES "YDFFLX" , "YNTFLX"
C      DO 230 J=1,NYP1
        DO 230 I=1,NX
          AVYVL(I,J)=DXGN(I+1)*DYGNH(J)
          NUYVOL(I,J)=NUY(I,J)*AVYVL(I,J)
          MUYVOL(I,J)=MUY(I,J)*AVYVL(I,J)
          TEMP4(I,J)=RHO(I+1,J+1,KO)-RHO(I+1,J,KO)
          YDFFLX(I,J)=NUYVOL(I,J)*TEMP4(I,J)
          TEMP4(I,J)=RHO(I+1,J+1,KN)-RHO(I+1,J,KN)
230      YNTFLX(I,J)=MUYVOL(I,J)*TEMP4(I,J)
C
C      ADD Y-DIFFUSION TO "CELMAS"
C      DO 240 J=1,NY
        DO 240 I=1,NX
          TEMP6(I,J)=YDFFLX(I,J+1)-YDFFLX(I,J)
240      CELMAS(I,J)=CELMAS(I,J)+TEMP6(I,J)
C
C      IF SYNCHRONIZATION OF ANTI-DIFFUSION FLUXES IS SPECIFIED, SKIP
C      EVALUATION OF CORRECTION FACTORS
        IF(SNKRNZ) GO TO 445
C
C
C      EVALUATE TRANSPORTED-DIFFUSED DENSITY
        DO 250 J=1,NY
          DO 250 I=1,NX
            RVOL(I,J)=RDXGN(I+1)*RDYGN(J+1)
250      RHO(I+1,J+1,KN)=CELMAS(I,J)*RVOL(I,J)
C
C      EVALUATE TRANSPORTED-DIFFUSED DENSITY AT BOTTOM AND TOP BOUNDARIES
C      DO 260 I=2,NXP1
        TEMP1(I,1)=1.0
        TEMP2(I-1,NYP1)=1.0
        RHO(I,1,KN)=PBC(I)*RHO(I,JB,KN)+RHOBBC(I)
260      RHO(I,NYP2,KN)=TBC(I)*RHO(I,JT,KN)+RHOTBC(I)
C
C      EVALUATE TRANSPORTED-DIFFUSED DENSITY AT LEFT AND RIGHT BOUNDARIES
C      DO 270 J=2,NYP1
        TEMP1(1,J)=1.0
        TEMP2(NXF1,J-1)=1.0
        RHO(1,J,KN)=LBC(J)*RHO(IL,J,KN)+RHOLEBC(J)
270      RHO(NXP2,J,KN)=RBC(J)*RHO(IR,J,KN)+RHORBC(J)
C
C

```



```

C      CANCEL THE ANTI-DIFFUSION X-FLUX IF IT IS OPPOSITE TO ITS LOCAL
C      TRANSPORTED-DIFFUSED DENSITY GRADIENT AND ANY OF THE ADJACENT ONES
      DO 280 J=1,NY
      DO 280 I=1,NXP1
280     DIFF(I,J)=RHO(I+1,J+1,KN)-RHO(I,J+1,KN)
C
      DO 290 J=1,NY
      DO 290 I=1,NX
      TEMP1(I+1,J+1)=XOR(XNTFLX(I+1,J),DIFF(I,J))
290     TEMP2(I,J)=XOR(XNTFLX(I,J),DIFF(I+1,J))
C
      DO 300 J=1,NY
      DO 300 I=1,NXP1
      TEMP5(I,J)=XOR(XNTFLX(I,J),DIFF(I,J))
      TEMP6(I,J)=OR(TEMP1(I,J+1),TEMP2(I,J))
      FLX(I,J)=AND(TEMP5(I,J),TEMP6(I,J))
      FLX(I,J)=COMPL(FLX(I,J))
      IFLX(I,J)=LSHF(IFLX(I,J),-31)
      FLX(I,J)=FLOAT(IFLX(I,J))
300     XNTFLX(I,J)=XNTFLX(I,J)*FLX(I,J)
C
C      IF X-COORDINATE IS PERIODIC AND EITHER LEFT OR RIGHT BOUNDARY'S
C      ANTI-DIFFUSION FLUX IS CANCELLED, CANCEL THE OTHER
      IF(.NOT.XPRDC) GO TO 305
C
      DO 304 J=1,NY
      XNTFLX(1,J)=AND(XNTFLX(1,J),XNTFLX(NXP1,J))
304     XNTFLX(NXP1,J)=XNTFLX(1,J)
C
305     CONTINUE
C
C
C      CANCEL THE ANTI-DIFFUSION Y-FLUX IF IT IS OPPOSITE TO ITS LOCAL
C      TRANSPORTED-DIFFUSED DENSITY GRADIENT AND ANY OF THE ADJACENT ONES
      DO 310 J=1,NYP1
      DO 310 I=1,NX
310     DIFF(I,J)=RHO(I+1,J+1,KN)-RHO(I+1,J,KN)
C
      DO 320 J=1,NY
      DO 320 I=1,NX
      TEMP1(I+1,J+1)=XOR(YNTFLX(I,J+1),DIFF(I,J))
320     TEMP2(I,J)=XOR(YNTFLX(I,J),DIFF(I,J+1))
C
      DO 330 J=1,NYP1
      DO 330 I=1,NX
      TEMP5(I,J)=XOR(YNTFLX(I,J),DIFF(I,J))
      TEMP6(I,J)=OR(TEMP1(I+1,J),TEMP2(I,J))
      FLX(I,J)=AND(TEMP5(I,J),TEMP6(I,J))
      FLX(I,J)=COMPL(FLX(I,J))
      IFLX(I,J)=LSHF(IFLX(I,J),-31)
      FLX(I,J)=FLOAT(IFLX(I,J))
330     YNTFLX(I,J)=YNTFLX(I,J)*FLX(I,J)
C

```

```

C      IF Y-COORDINATE IS PERIODIC AND EITHER BOTTOM OR TOP BOUNDARY'S
C      ANTI-DIFFUSION FLUX IS CANCELLED, CANCEL THE OTHER
C      IF(.NOT.YPRDC) GO TO 335
C
C      DO 334 I=1,NX
C      YNTFLX(I,1)=AND(YNTFLX(I,1),YNTFLX(I,NYP1))
334    YNTFLX(I,NYP1)=YNTFLX(I,1)
C
C      335    CONTINUE
C
C
C      EVALUATE NET INCOMING "FLXIN", OUTGOING "FLXOUT" ANTI-DIFFUSION
C      DO 340 J=1,NY
C      DO 340 I=1,NXP1
C      TEMP5(I,J)=ASHF(XNTFLX(I,J),-31)
C      MNFLX(I,J)=AND(XNTFLX(I,J),TEMP5(I,J))
C      TEMP5(I,J)=XOR(XNTFLX(I,J),TEMP5(I,J))
340    MXFLX(I,J)=AND(XNTFLX(I,J),TEMP5(I,J))
C
C      DO 350 J=1,NY
C      DO 350 I=1,NX
C      FLXIN(I+1,J+1)=1.E-50+MXFLX(I,J)
C      FLXOUT(I+1,J+1)=1.E-50-MNFLX(I,J)
C      FLXIN(I+1,J+1)=FLXIN(I+1,J+1)-MNFLX(I+1,J)
350    FLXOUT(I+1,J+1)=FLXOUT(I+1,J+1)+MXFLX(I+1,J)
C
C      DO 360 J=1,NYP1
C      DO 360 I=1,NX
C      TEMP5(I,J)=ASHF(YNTFLX(I,J),-31)
C      MNFLX(I,J)=AND(YNTFLX(I,J),TEMP5(I,J))
C      TEMP5(I,J)=XOR(YNTFLX(I,J),TEMP5(I,J))
360    MXFLX(I,J)=AND(YNTFLX(I,J),TEMP5(I,J))
C
C      DO 370 J=1,NY
C      DO 370 I=1,NX
C      FLXIN(I+1,J+1)=FLXIN(I+1,J+1)+MXFLX(I,J)
C      FLXOUT(I+1,J+1)=FLXOUT(I+1,J+1)-MNFLX(I,J)
C      FLXIN(I+1,J+1)=FLXIN(I+1,J+1)-MNFLX(I,J+1)
370    FLXOUT(I+1,J+1)=FLXOUT(I+1,J+1)+MXFLX(I,J+1)
C
C
C      GO TO (375,385) ILMTR
C
C      375    CONTINUE
C      IF BORIS-BOOK FLUX LIMITER IS REQUESTED, USE TRANSPORTED-DIFFUSED
C      DENSITY TO BOUND NEW DENSITY
C      DO 380 J=1,NYP2
C      DO 380 I=1,NXP2
380    TEMP5(I,J)=RHO(I,J,KN)
C
C      GO TO 395
C

```

```

385     CONTINUE
C     IF ZALESK FLUX LIMITER IS REQUESTED, USE MAXIMUM OF OLD AND
C     TRANSPORTED-DIFFUSED DENSITY AS UPPER BOUND FOR NEW DENSITY
        DO 390 J=1,NYP2
        DO 390 I=1,NXP2
390     TEMP5(I,J)=AMAX1(RHO(I,J,KO),RHO(I,J,KN))
C
395     CONTINUE
C
        DO 400 J=2,NYP1
C     EVALUATE MAXIMUM ADMISSIBLE ANTI-DIFFUSION INTO CELL "MXIN", AND
C     IN TURN CORRECTION FACTOR "RIN"
        DO 400 I=2,NXP1
            TEMP6(I,J)=AMAX1(TEMP5(I,J),TEMP5(I-1,J))
            TEMP6(I,J)=AMAX1(TEMP6(I,J),TEMP5(I+1,J))
            TEMP6(I,J)=AMAX1(TEMP6(I,J),TEMP5(I,J-1))
            RHOMX(I,J)=AMAX1(TEMP6(I,J),TEMP5(I,J+1))
            TEMP6(I,J)=RHOMX(I,J)-RHO(I,J,KN)
            TEMP6(I,J)=TEMP6(I,J)*DXGN(I)
            MXIN(I,J)=TEMP6(I,J)*DYGN(J)
            TEMP6(I,J)=MXIN(I,J)/FLXIN(I,J)
400     RIN(I,J)=AMIN1(1.0,TEMP6(I,J))
C
        GO TO (415,405) ILMTR
C
405     CONTINUE
C     IF ZALESK FLUX LIMITER IS REQUESTED, USE MINIMUM OF OLD AND
C     TRANSPORTED-DIFFUSED DENSITY AS LOWER BOUND FOR NEW DENSITY
        DO 410 J=1,NYP2
        DO 410 I=1,NXP2
410     TEMP5(I,J)=AMIN1(RHO(I,J,KO),RHO(I,J,KN))
C
415     CONTINUE
C     EVALUATE MAXIMUM ADMISSIBLE ANTI-DIFFUSION OUT OF CELL "MXOUT",
C     AND IN TURN CORRECTION FACTOR "ROUT"
        DO 420 J=2,NYP1
        DO 420 I=2,NXP1
            TEMP6(I,J)=AMIN1(TEMP5(I,J),TEMP5(I-1,J))
            TEMP6(I,J)=AMIN1(TEMP6(I,J),TEMP5(I+1,J))
            TEMP6(I,J)=AMIN1(TEMP6(I,J),TEMP5(I,J-1))
            RHOMN(I,J)=AMIN1(TEMP6(I,J),TEMP5(I,J+1))
            TEMP6(I,J)=RHO(I,J,KN)-RHOMN(I,J)
            TEMP6(I,J)=TEMP6(I,J)*DXGN(I)
            MXOUT(I,J)=TEMP6(I,J)*DYGN(J)
            TEMP6(I,J)=MXOUT(I,J)/FLXOUT(I,J)
420     ROUT(I,J)=AMIN1(1.0,TEMP6(I,J))
C

```

```

C      IF A COORDINATE IS NOT PERIODIC, "RIN", ROUT " ARE ASSUMED TO BE
C      CONTINUOUS THROUGH ITS NORMAL BOUNDARY
      DO 430 I=2,NXP1
      RIN(I,1)=RIN(I,JB)
      RIN(I,NYP2)=RIN(I,JT)
      ROUT(I,1)=ROUT(I,JB)
430    ROUT(I,NYP2)=ROUT(I,JT)
C
      DO 440 J=2,NYP1
      RIN(1,J)=RIN(IL,J)
      RIN(NXP2,J)=RIN(IR,J)
      ROUT(1,J)=ROUT(IL,J)
440    ROUT(NXP2,J)=ROUT(IR,J)
C
445    CONTINUE
C
C
C      LIMIT ANTI-DIFFUSION FLUXES USING MINIMUM OF ADJACENT CELLS'
C      MAXIMUM ADMISSIBLE FLUXES
      DO 450 J=1,NY
      DO 450 I=1,NXP1
      FLX(I,J)=XNTFLX(I,J)
      IFLX(I,J)=LSHF(IFLX(I,J),-31)
      FLX(I,J)=FLOAT(IFLX(I,J))
      RHO(I+1,J+1,KN)=AMIN1(RIN(I,J+1),ROUT(I+1,J+1))
      XFLXCR(I,J)=FLX(I,J)*RHO(I+1,J+1,KN)
      RHO(I+1,J+1,KN)=AMIN1(RIN(I+1,J+1),ROUT(I,J+1))
      FLX(I,J)=1.0-FLX(I,J)
      FLX(I,J)=FLX(I,J)*RHO(I+1,J+1,KN)
      XFLXCR(I,J)=XFLXCR(I,J)+FLX(I,J)
450    XNTFLX(I,J)=XNTFLX(I,J)*XFLXCR(I,J)
C
      DO 460 J=1,NYP1
      DO 460 I=1,NX
      FLX(I,J)=YNTFLX(I,J)
      IFLX(I,J)=LSHF(IFLX(I,J),-31)
      FLX(I,J)=FLOAT(IFLX(I,J))
      RHO(I+1,J+1,KN)=AMIN1(RIN(I+1,J),ROUT(I+1,J+1))
      YFLXCR(I,J)=FLX(I,J)*RHO(I+1,J+1,KN)
      RHO(I+1,J+1,KN)=AMIN1(RIN(I+1,J+1),ROUT(I+1,J))
      FLX(I,J)=1.0-FLX(I,J)
      FLX(I,J)=FLX(I,J)*RHO(I+1,J+1,KN)
      YFLXCR(I,J)=YFLXCR(I,J)+FLX(I,J)
460    YNTFLX(I,J)=YNTFLX(I,J)*YFLXCR(I,J)
C
C

```

```

C      ADD CORRECTED ANTI-DIFFUSION FLUXES AND EVALUATE NEW DENSITY
      DO 470 J=1,NY
      DO 470 I=1,NX
      TEMP5(I,J)=XNTFLX(I,J)-XNTFLX(I+1,J)
      TEMP6(I,J)=YNTFLX(I,J)-YNTFLX(I,J+1)
      CELMAS(I,J)=CELMAS(I,J)+TEMP5(I,J)
      CELMAS(I,J)=CELMAS(I,J)+TEMP6(I,J)
      RVOL(I,J)=RDXGN(I+1)*RDIYGN(J+1)
470    RHO(I+1,J+1,KR)=CELMAS(I,J)*RVOL(I,J)
C
C      EVALUATE NEW DENSITY AT BOTTOM AND TOP BOUNDARIES
      DO 490 I=2,NXP1
      RHO(I,1,KR)=BBC(I)*RHO(I,JB,KR)+RHOBBC(I)
490    RHO(I,NYP2,KR)=TBC(I)*RHO(I,JT,KR)+RHOTBC(I)
C
C      EVALUATE NEW DENSITY AT LEFT AND RIGHT BOUNDARIES
      DO 500 J=2,NYP1
      RHO(1,J,KR)=LBC(J)*RHO(IL,J,KR)+RHO LBC(J)
500    RHO(NXP2,J,KR)=RBC(J)*RHO(IR,J,KR)+RHO RBC(J)
C
C      RETURN
C
C
C

```

ENTRY NGRID(XGN,YGN)  
-----

EVALUATE AVERAGE ( BETWEEN OLD AND NEW ) INTERFACE VELOCITY AND AREA  
AND NEW AND AVERAGE VOLUME COMPONENTS.  
IF X-GRID OR Y-GRID IS NOT MOVING, USE ITS OLD VALUES.  
INTERFACE VOLUME IS CONSIDERED AVERAGE OF ADJACENT CELLS' VOLUMES.

GO TO (510,520,530,540,550,560,570) GEOM

510 CONTINUE

CARTESIAN COORDINATES

IF(.NOT.XCHNG) GO TO 513

DO 511 I=1,NXP1  
XG(I)=0.5\*(XGN(I)+XGO(I))  
511 DXG(I)=XGN(I)-XGO(I)

DO 512 I=2,NXP1  
DXGN(I)=XGN(I)-XGN(I-1)  
AX(I-1)=XG(I)-XG(I-1)  
512 RDXGN(I)=1.0/DXGN(I)

513 CONTINUE  
IF(.NOT.YCHNG) GO TO 580

DO 516 J=1,NYP1  
YG(J)=0.5\*(YGN(J)+YGO(J))  
516 DYG(J)=YGN(J)-YGO(J)

DO 517 J=2,NYP1  
DYGN(J)=YGN(J)-YGN(J-1)  
AY(J-1)=YG(J)-YG(J-1)  
517 RDYGN(J)=1.0/DYGN(J)

GO TO 580

520 CONTINUE

CYLINDRICAL R-Z COORDINATES

IF(.NOT.XCHNG) GO TO 523

DO 521 I=1,NXP1  
SQO(I)=0.5\*(XGO(I)\*XGO(I))  
SQN(I)=0.5\*(XGN(I)\*XGN(I))  
XG(I)=SQN(I)+SQO(I)  
DXG(I)=SQN(I)-SQO(I)  
521 SQ(I)=SQRT(XG(I))

```

      DO 522 I=2,NXP1
      DXGN(I)=SQN(I)-SQN(I-1)
      AX(I-1)=0.5*(XG(I)-XG(I-1))
522   RDXGN(I)=1.0/DXGN(I)
C
523   CONTINUE
      IF(.NOT.YCHNG) GO TO 580
C
      DO 526 J=1,NYP1
      YG(J)=0.5*(YGN(J)+YGO(J))
526   DYG(J)=YGN(J)-YGO(J)
C
      DO 527 J=2,NYP1
      DYGN(J)=YGN(J)-YGN(J-1)
      AY(J-1)=YG(J)-YG(J-1)
527   RDYGN(J)=1.0/DYGN(J)
C
      GO TO 580
C
530   CONTINUE
C   CYLINDRICAL R-FYE COORDINATES
540   CONTINUE
C   CYLINDRICAL Z-FYE COORDINATES
550   CONTINUE
C   SPHERICAL R-THETA COORDINATES
560   CONTINUE
C   SPHERICAL R-FYE COORDINATES
570   CONTINUE
C   SPHERICAL THETA-FYE COORDINATES
C
      PRINT 70
      STOP
C

```

```

580      CONTINUE
        IF (.NOT.XCHNG) GO TO 586
C
        DXGN(1)=DXGN(IL)
        DXGN(NXP2)=DXGN(IR)
        RDXGN(1)=RDXGN(IL)
        RDXGN(NXP2)=RDXGN(IR)
C
        DO 585 I=1,NXP1
        DXGNH(I)=0.5*(DXGN(I)+DXGN(I+1))
585      RDXGNH(I)=0.5*(RDXGN(I)+RDXGN(I+1))
C
586      CONTINUE
        IF (.NOT.YCHNG) RETURN
C
        DYGN(1)=DYGN(JB)
        DYGN(NYP2)=DYGN(JT)
        RDYGN(1)=RDYGN(JB)
        RDYGN(NYP2)=RDYGN(JT)
C
        DO 590 J=1,NYP1
        DYGNH(J)=0.5*(DYGN(J)+DYGN(J+1))
590      RDYGNH(J)=0.5*(RDYGN(J)+RDYGN(J+1))
C
        RETURN
C
C
C

```



```

C      ENTRY OGRID(XGN,YGN)
C      -----
C      RESET OLD GRID PARAMETERS, IN PREPARATION FOR A NEW TIME STEP
C
C      IF(.NOT.XCHNG) GO TO 593
C
C      DO 592 I=1,NXP2
592    DXGO(I)=DXGN(I)
C
C      593    CONTINUE
C      IF(.NOT.YCHNG) GO TO 595
C
C      DO 594 J=1,NYP2
594    DYGO(J)=DYGN(J)
C
C      GO TO 595
C
C
C      ENTRY ORIGRD(XGN,YGN)
C      -----
C      ORIGINATE THE GRID
C
C      SET DEFAULT : GRID IS MOVING
C      XCHNG=.TRUE.
C      YCHNG=.TRUE.
C
C      595    CONTINUE
C      IF(.NOT.XCHNG) GO TO 597
C
C      DO 596 I=1,NXP1
596    XGO(I)=XGN(I)
C
C      597    CONTINUE
C      IF(.NOT.YCHNG) RETURN
C
C      DO 598 J=1,NYP1
598    YGO(J)=YGN(J)
C
C      RETURN
C
C
C

```

ENTRY VOLFLX(U,V,DT)

EVALUATE X AND Y VOLUMETRIC FLUX THROUGH INTERFACES

DT2=0.5\*DT

DO 602 J=1,NY

DO 602 I=1,NXP1

602 ADUDT(I,J)=U(I,J+1)+U(I+1,J+1)

DO 604 J=1,NYP1

DO 604 I=1,NX

604 ADVDT(I,J)=V(I+1,J)+V(I+1,J+1)

GO TO (610,620,630,640,650,660,670) GEOM

610 CONTINUE

CARTESIAN COORDINATES

DO 611 J=1,NY

DO 611 I=1,NXP1

ADUDT(I,J)=ADUDT(I,J)\*DT2

ADUDT(I,J)=ADUDT(I,J)-DXG(I)

611 ADUDT(I,J)=ADUDT(I,J)\*AY(J)

DO 612 J=1,NYP1

DO 612 I=1,NX

ADVDT(I,J)=ADVDT(I,J)\*DT2

ADVDT(I,J)=ADVDT(I,J)-DYG(J)

612 ADVDT(I,J)=ADVDT(I,J)\*AX(I)

RETURN

620 CONTINUE

CYLINDRICAL R-Z COORDINATES

DO 621 J=1,NY

DO 621 I=1,NXP1

ADUDT(I,J)=ADUDT(I,J)\*SQ(I)\*DT2

ADUDT(I,J)=ADUDT(I,J)-DXG(I)

621 ADUDT(I,J)=ADUDT(I,J)\*AY(J)

DO 622 J=1,NYP1

DO 622 I=1,NX

ADVDT(I,J)=ADVDT(I,J)\*DT2

ADVDT(I,J)=ADVDT(I,J)-DYG(J)

622 ADVDT(I,J)=ADVDT(I,J)\*AX(I)

RETURN

630 CONTINUE  
C CYLINDRICAL R-FYE COORDINATES  
640 CONTINUE  
C CYLINDRICAL Z-FYE COORDINATES  
650 CONTINUE  
C SPHERICAL R-THETA COORDINATES  
660 CONTINUE  
C SPHERICAL R-FYE COORDINATES  
670 CONTINUE  
C SPHERICAL THETA-FYE COORDINATES  
C

PRINT 70  
STOP

C  
C  
C

ENTRY SORCES(SRCTYP,SORCE,DT)  
-----

MANAGEMENT OF SOURCE TERM EVALUATION

IF(SRCTYP.EQ.BDF) GO TO 750

IF(SRCTYP.EQ.XGRD) GO TO (760,800,999,999,999,999,999) GEOM

IF(SRCTYP.EQ.YGRD) GO TO (780,780,999,999,999,999,999) GEOM

IF(SRCTYP.EQ.DIV) GO TO (760,950,999,999,999,999,999) GEOM

TEXT(6)=TEXT(18)

TEXT(7)=TEXT(19)

TEXT(8)=TEXT(20)

PRINT 10, (TEXT(I),I=1,11)

STOP

ENTRY CLR SRC  
-----

CLEAR SOURCE TERM

LSRC=.FALSE.

DO 710 J=1,NY

DO 710 I=1,NX

710 SOURCE(I,J)=0.

RETURN

ENTRY BODY(SORCE,DT)  
-----

EVALUATE BODY FORCE TYPE SOURCE TERMS

750 CONTINUE

LSRC=.TRUE.

DO 755 J=1,NY

DO 755 I=1,NX

TEMP3(I,J)=AX(I)\*AY(J)

TEMP4(I,J)=SORCE(I+1,J+1)\*DT

TEMP5(I,J)=TEMP3(I,J)\*TEMP4(I,J)

755 SOURCE(I,J)=SOURCE(I,J)+TEMP5(I,J)

RETURN

```

      ENTRY XGRAD(SORCE,DT)
      -----
C
C
C      EVALUATE  CARTESIAN X GRADIENT COMPONENT
      SRCTYP=XGRD
760      CONTINUE
      LSRC=.TRUE.
      DT2=0.5*DT
C
      DO 765 J=1,NY
      DO 765 I=1,NXP1
765      TEMP3(I,J)=SORCE(I,J+1)+SORCE(I+1,J+1)
C
      DO 770 J=1,NY
      DO 770 I=1,NX
      TEMP4(I,J)=TEMP3(I+1,J)-TEMP3(I,J)
      TEMP5(I,J)=TEMP4(I,J)*AY(J)*DT2
770      SOURCE(I,J)=SOURCE(I,J)+TEMP5(I,J)
C
      IF(SRCTYP.EQ.DIV) GO TO 780
C
      RETURN
C
C
C
      ENTRY YGRAD(SORCE,DT)
      -----
C
C
C      EVALUATE  CARTESIAN Y GRADIENT COMPONENT
780      CONTINUE
      LSRC=.TRUE.
      DT2=0.5*DT
C
      DO 785 J=1,NYP1
      DO 785 I=1,NX
785      TEMP3(I,J)=SORCE(I+1,J)+SORCE(I+1,J+1)
C
      DO 790 J=1,NY
      DO 790 I=1,NX
      TEMP4(I,J)=TEMP3(I,J+1)-TEMP3(I,J)
      TEMP5(I,J)=TEMP4(I,J)*AX(I)*DT2
790      SOURCE(I,J)=SOURCE(I,J)+TEMP5(I,J)
C
      RETURN
C
C
C

```

```

      ENTRY RCGRAD(SORCE,DT)
      -----
C
C
C    EVALUATE CYLINDRICAL R GRADIENT COMPONENT
800    CONTINUE
      LSRC=.TRUE.
C
      DO 805 J=1,NY
      DO 805 I=1,NXP1
      TEMP3(I,J)=SORCE(I,J+1)+SORCE(I+1,J+1)
      TEMP4(I,J)=SQ(I)*AY(J)*DT
805    TEMP3(I,J)=0.5*TEMP3(I,J)
C
      DO 810 J=1,NY
      DO 810 I=1,NX
      TEMP3(I,J)=TEMP3(I,J)*TEMP4(I+1,J)
810    TEMP5(I,J)=TEMP4(I+1,J)-TEMP4(I,J)
C
      DO 815 J=1,NY
      DO 815 I=1,NX
      TEMP4(I,J)=TEMP3(I+1,J)-TEMP3(I,J)
      TEMP5(I,J)=TEMP5(I,J)*SORCE(I+1,J+1)
      SOURCE(I,J)=SOURCE(I,J)+TEMP4(I,J)
815    SOURCE(I,J)=SOURCE(I,J)+TEMP5(I,J)
C
      RETURN
C
C
C
      ENTRY RCDIV(SORCE,DT)
      -----
C
C
C    EVALUATE CYLINDRICAL DIVERGENCE
950    CONTINUE
      LSRC=.TRUE.
      DT2=0.5*DT
C
      DO 955 J=1,NY
      DO 955 I=1,NXP1
      TEMP3(I,J)=SORCE(I,J+1)+SORCE(I+1,J+1)
955    TEMP4(I,J)=SQ(I)*AY(J)*DT2
C
      DO 960 J=1,NY
      DO 960 I=1,NX
      TEMP5(I,J)=TEMP3(I+1,J)-TEMP3(I,J)
      TEMP3(I,J)=TEMP5(I,J)*TEMP4(I+1,J)
960    SOURCE(I,J)=SOURCE(I,J)+TEMP3(I,J)
C
      GO TO 780
C
      RETURN
C
999    PRINT 70
      STOP
C
C
C

```

```

C      ENTRY SETGOM(GOMTRY,CRD1,CRD2,N1,N2)
C      -----
C      SET AND CHECK REQUEST FOR A PARTICULAR GEOMETRY
C
C      GEOM=0
C
C      IF(GOMTRY.EQ.TGM(1)) GEOM=1
C
C      IF(GOMTRY.NE.TGM(2)) GO TO 1210
C      IF(CRD1.NE.TCRD(4)) GO TO 1205
C      IF(CRD2.EQ.TCRD(3)) GEOM=2
C      IF(CRD2.EQ.TCRD(6)) GEOM=3
1205  CONTINUE
C      IF(CRD1.EQ.TCRD(3).AND.CRD2.EQ.TCRD(6)) GEOM=4
C
1210  CONTINUE
C      IF(GOMTRY.NE.TGM(3)) GO TO 1220
C      IF(CRD1.NE.TCRD(4)) GO TO 1215
C      IF(CRD2.EQ.TCRD(5)) GEOM=5
C      IF(CRD2.EQ.TCRD(6)) GEOM=6
1215  CONTINUE
C      IF(CRD1.EQ.TCRD(5).AND.CRD2.EQ.TCRD(6)) GEOM=7
C
1220  CONTINUE
C      IF(GEOM.GT.0) GO TO 1225
C
C      ISSUE AN ERROR MESSAGE UPON REQUEST OF AN UNRECOGNIZED GEOMETRY
C      AND STOP
C      TEXT(6)=TEXT(12)
C      TEXT(7)=TEXT(13)
C      TEXT(8)=TEXT(14)
C      PRINT 10, (TEXT(I),I=1,11)
C
C      STOP
C
1225  CONTINUE
C
C      NX=N1
C      NXP1=NX+1
C      NXP2=NX+2
C
C      NY=N2
C      NYP1=NY+1
C      NYP2=NY+2
C
C      XPRDC=.FALSE.
C      IL=2
C      IR=NXP1
C
C      YPRDC=.FALSE.
C      JB=2
C      JT=NYP1
C
C      LSRC=.FALSE.

```

```
C      SET DEFAULT : ALL BOUNDARIES ASSUMED PERMEABLE
      DO 1226 I=1,NXP2
      FRMBLB(I)=1.0
1226   FRMBLT(I)=1.0
C
      DO 1227 J=1,NYP2
      FRMBLL(J)=1.0
1227   FRMBLR(J)=1.0
C
      PRINT 30
C
      RETURN
C
C
C
```



```
ENTRY PRODIC(CRONT,CRD)
```

IDENTIFY X OR Y COORDINATE AS PERIODIC

```
IF (CRONT.NE.1) GO TO 1230
```

```
XPRDC=.TRUE.
```

IR=2

$$IL = NXF \cdot 1$$

PRINT 40, CRD

CONTINUE

```
IF (CRONT.NE.2) GO TO 1240
```

```
YPRDC=.TRUE.
```

**JT=2**

JB=NYP 1

PRINT 40, CRD

CONTINUE

```
IF (CRD.EQ.TCRD(4).OR.CRD.EQ.TCRD(5)) PRINT 20,CRD
```

RETURN

```

      ENTRY SETLMT(LMTR1,LMTR2)
      -----
C
C
C      SET AND CHECK REQUEST FOR A PARTICULAR FLUX LIMITER
C
C      DO 1255 I=1,4
C
C      DO 1251 J=1,2
      IF(LMTR1(J).NE.TLM1(J,I)) GO TO 1255
1251      CONTINUE
C
C      DO 1252 J=1,2
      IF(LMTR2(J).NE.TLM2(J,I)) GO TO 1255
1252      CONTINUE
C
C      GO TO 1260
C
C      1255      CONTINUE
C
C      ISSUE AN ERROR MESSAGE UPON REQUEST OF AN UNRECOGNIZED FLUX
C      LIMITER AND STOP
      TEXT(6)=TEXT(15)
      TEXT(7)=TEXT(16)
      TEXT(8)=TEXT(17)
      PRINT 10, (TEXT(I),I=1,11)
C
C      STOP
C
C      1260      CONTINUE
      ILMTR=I
C
C      RETURN
C
C
C

```

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```
IF (BONDY.NE.TBND(1)) GO TO 1280
```

1275

```
PRINT 60, BONDY,KSTRT,KEND
```

1280

DO 1285 J=KSTRT,KEND

1285

CONTINUE

1290

1295

```
PRINT 60, BONDRY, KSTRT, KEND
```

1300

```
DO 1305 I=KSTRT,KEND
```

1305

CONTINUE

END

```

C      SUBROUTINE NUMU(NI,NJ,EPS,NUV,MUV)
C
C      EVALUATE  DIFFUSION AND ANTI-DIFFUSION COEFFICIENTS
C
C      PARAMETER      NPX=100,NPY=100
C      PARAMETER      NP1X=NPX+1,NP1Y=NPY+1
C      PARAMETER      NP2X=NPX+2,NP2Y=NPY+2
C
C      REAL      EPS(NP1X,NP1Y),NUV(NP2X,NP2Y),MUV(NP2X,NP2Y)
C
C      DO 100 J=1,NJ
C      DO 100 I=1,NI
C      EPS(I,J)=EPS(I,J)*EPS(I,J)
C      NUV(I,J)=0.333333*EPS(I,J)
C      NUV(I,J)=0.166667+NUV(I,J)
C      MUV(I,J)=NUV(I,J)-EPS(I,J)
C
C      RETURN
C      END
100

```